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FULL PUBLICATION LIST

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Highly Cited Researcher by Clarivate Analytics 2018, H-index = 67 (WoS May 2020)

The 10 most significant publications, relevant for PI's current research:

1. O. Lopez-Acevedo, K.A. Kacprzak, J. Akola, **H. Häkkinen**, "Quantum size effects in ambient CO oxidation catalysed by ligand-protected gold clusters", *Nature Chem.* 2, 329 (2010).
2. **H. Häkkinen**, "The gold-sulfur interface at the nanoscale", *Nature Chem.* 4, 443 (2012). An invited review, WoS "highly cited" paper. It was listed in top-10 most cited papers in Nature Chemistry in 2016 by Google Scholar.
3. H.Yang, Y. Wang, H. Huang, L. Gell, L. Lehtovaara, S. Malola, **H. Häkkinen**, N. Zheng, "All- thiol-stabilized Ag44 and Au12Ag32 nanoparticles with single-crystal structures", *Nature Comm.* 4, 2422 (2013). WoS "highly cited" paper.
4. V. Marjomäki, T. Lahtinen, M. Martikainen, J. Koivisto, S. Malola, K. Salorinne, M. Pettersson, **H. Häkkinen**, "Site-specific targeting of enterovirus capsid by functionalized monodisperse gold nanoclusters", *Proc. Natl. Acad. Sci. (USA)* 111, 1277 (2014).
5. M. Azubel, J. Koivisto, S. Malola, D. Bushnell, G.L. Hura, A.L. Koh, H. Tsunoyama, T. Tsukuda, M. Pettersson, **H. Häkkinen**, R.D. Kornberg, "Electron microscopy of gold nanoparticles at atomic resolution", *Science* 345, 909 (2014). WoS "highly cited" paper.
6. K. Salorinne, S. Malola, O.A. Wong, C.D. Rithner, X. Chen, C.J. Ackerson, **H. Häkkinen**, "Conformation and dynamics of the ligand shell of a water-soluble Au102 nanoparticle", *Nature Comm.* 7, 10401 (2016).
7. H. Yang, Y. Wang, X. Chen, X. Zhao, L. Gu, H. Huang, J. Yan, C. Xu, G. Li, J. Wu, A.J. Edwards, B. Dittrich, Z. Tang, D. Wang, L. Lehtovaara, **H. Häkkinen** and N.F. Zheng, "Plasmonic twinned silver nanoparticles with molecular precision", *Nature Comm.* 7, 12809 (2016).
8. Q. Zhou, S. Kaappa, S. Malola, H. Lu, D. Guan, Y. Li, H. Wang, Z. Xie, Z. Ma, **H. Häkkinen**, N. Zheng, X. Yang, L. Zheng, "Real-Space Imaging with Pattern Recognition of a Ligand-Protected Ag374 Nanocluster at Sub-Molecular Resolution", *Nature Comm.* 9, 2948 (2018).
9. M.R. Narouz, P.J. Unsworth, K. Salorinne, S. Takano, R. Tomihara, S. Kaappa, S. Malola, C.T. Dingh, J.D. Padmos, K. Ayoo, P.J. Garrett, M. Nambo, J. Hugh Horton, E.H. Sargent, **H. Häkkinen**, T. Tsukuda, C.M. Crudden, "N-Heterocyclic Carbene-Functionalized Magic Number Gold Nanoclusters", *Nature Chem.* 11, 419 (2019) (cover article 5/2019).
10. S. Malola, P. Nieminen, A. Pihlajamäki, J. Hämäläinen, T. Kärkkäinen, **H. Häkkinen**, "A method for structure prediction of metal-ligand interfaces of hybrid nanoparticles", *Nature Comm.* 2019 DOI: 10.1038/s41467-019-12031-w

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A. Peer-reviewed scientific articles

- (1) **H. Häkkinen**, S. Mäkinen and M. Manninen, "Positron states in dislocations: Shallow and deep traps", *Europhys. Lett.* **9**, 809-814 (1989).
- (2) **H. Häkkinen** and M. Manninen, "The effective-medium theory beyond the nearest-neighbour interaction", *J. Phys.: Condens. Matter* **1**, 9765-9777 (1989).
- (3) **H. Häkkinen**, S. Mäkinen and M. Manninen, "Edge dislocations in fcc-metals: Microscopic calculations of core structure and positron states in Al and Cu", *Phys. Rev. B* **41**, 12441-12453 (1990).
- (4) **H. Häkkinen**, J. Merikoski and M. Manninen, "Surface reconstruction and many-atom models", *J. Phys.: Condens. Matter* **3**, 2755-2767 (1991).
- (5) **H. Häkkinen**, J. Mansikka-aho and M. Manninen, "From the Huckel model to effective-medium theory", *J. Phys.: Condens. Matter* **3**, 7757-7762 (1991).
- (6) M. Manninen and **H. Häkkinen**, "A method for detecting vacancy diffusion in molecular dynamics", *J. Comp. Phys.* **100**, 197-199 (1992).
- (7) **H. Häkkinen** and M. Manninen, "Computer simulation of disordering and premelting of low-index faces of copper", *Phys. Rev. B* **46**, 1725-1742 (1992).
- (8) **H. Häkkinen**, J. Merikoski, M. Manninen, J. Timonen and K. Kaski, "Roughening of the Cu(110) surface", *Phys. Rev. Lett.* **70**, 2451-2454 (1993).
- (9) **H. Häkkinen** and Uzi Landman, "Superheating, melting and annealing of copper surfaces", *Phys. Rev. Lett.* **71**, 1023-1026 (1993).
- (10) J. Merikoski, **H. Häkkinen**, M. Manninen, J. Timonen and K. Kaski, "Roughening of the Cu(110) surface", *Phys. Rev. B* **49**, 4938-4947 (1994).
- (11) **H. Häkkinen**, R. N. Barnett and U. Landman, "Metallization of the Na₁₄Cl₁₃ cluster", *Europhys. Lett.* **28**, 263-269 (1994).
- (12) **H. Häkkinen**, R. N. Barnett and U. Landman, "Energetics, structure and excess electrons in small sodium-chloride clusters", *Chem. Phys. Lett.* **232**, 79-89 (1995).
- (13) R. N. Barnett, H.-P. Cheng, **H. Häkkinen** and U. Landman, "Studies of excess electrons in sodium chloride clusters and of excess protons in water clusters", *J. Phys. Chem.* **99**, 7731-7753 (1995).
- (14) A. Landa, P. Wynblatt, **H. Häkkinen**, R. N. Barnett and U. Landman, "Equilibrium interphase interfaces and premelting of the Pb(110) surface", *Phys. Rev. B* **51**, 10972-10980 (1995).
- (15) **H. Häkkinen** and M. Manninen, "Electronic-structure-induced deformations of liquid metal clusters", *Phys. Rev. B* **52**, 1540-1543 (1995).
- (16) **H. Häkkinen** and M. Manninen, "Metallic clusters on an ionic surface", *Europhys. Lett.* **34**, 177-182 (1996).
- (17) **H. Häkkinen** and M. Manninen, "How 'magic' is a magic metal cluster?", *Phys. Rev. Lett.* **76**, 1599-1602 (1996).
- (18) **H. Häkkinen** and M. Manninen, "An *ab initio* study of cluster – surface interaction: Na clusters on the NaCl(001) surface", *J. Chem. Phys.* **105**, 10565-10571 (1996).

- (19) J. Kolehmainen, **H. Häkkinen** and M. Manninen, "Metal clusters on an inert surface: A simple model", Z. Phys. D **40**, 306-309 (1997).
- (20) **H. Häkkinen**, J. Kolehmainen, M. Koskinen, P. O. Lipas and M. Manninen, "Universal shapes of small fermion clusters", Phys. Rev. Lett. **78**, 1034-1037 (1997).
- (21) J. Kolehmainen, M. Koskinen, **H. Häkkinen** and M. Manninen, "Linear nuclei: A density-functional interpretation", Int. J. Mod. Phys. E **6**, 507-513 (1997).
- (22) S. M. Reimann, M. Koskinen, **H. Häkkinen**, P. E. Lindelof and M. Manninen, "Magic triangular and tetrahedral clusters", Phys. Rev. B **56**, 12147 (1997).
- (23) P. Heino, **H. Häkkinen** and K. Kaski, "Molecular dynamics study of mechanical properties of copper", Europhys. Lett. **41**, 278 (1998).
- (24) P. Heino, **H. Häkkinen** and K. Kaski, "Molecular dynamics study of copper with defects under strain", Phys. Rev. B **58**, 641-652 (1998).
- (25) A. Rytkönen, **H. Häkkinen** and M. Manninen, "Melting and octupole deformation of Na₄₀", Phys. Rev. Lett. **80**, 3940-3943 (1998).
- (26) J. Akola, **H. Häkkinen** and M. Manninen, "Ionization potential of Al clusters", Phys. Rev. B **58**, 3601-3604 (1998).
- (27) **H. Häkkinen** and M. Manninen, "Force fluctuations and localized states at point contacts", Europhys. Lett. **44**, 80-84 (1998).
- (28) A. Landa, **H. Häkkinen**, R. N. Barnett, P. Wynblatt, and U. Landman, "Disordering of the Pb(110) surface", Comp. Mater. Sci **11**, 245-251 (1998).
- (29) **H. Häkkinen**, R. N. Barnett and U. Landman, "Electronic structure of passivated Au₃₈(SCH₃)₂₄ nanocrystal", Phys. Rev. Lett. **82**, 3264-3267 (1999).
- (30) J. Akola, A. Rytkönen, **H. Häkkinen** and M. Manninen, "Temperature-dependent ionization potential of sodium clusters", Europ. Phys. J D **8**, 93-99 (2000).
- (31) J. Akola, M. Manninen, **H. Häkkinen**, U. Landman, X. Li, and L.-S. Wang, "Photoelectron Spectra of Aluminum Cluster Anions: Temperature Effects and Ab-Initio Simulations", Phys. Rev. B **60**, R11297-11300 (1999).
- (32) **H. Häkkinen**, R. N. Barnett, and U. Landman, "Gold Nanowires and their Chemical Modifications", J. Phys. Chem. B **103**, 8814-8816 (1999).
- (33) A. Sanchez, S. Abbet, U. Heiz, W.-D. Schneider, **H. Häkkinen**, R. N. Barnett, and U. Landman, "When Gold is not Noble: Nanoscale Gold Catalysts", J. Phys. Chem. A **103**, 9573 (1999).
- (34) J. Akola, **H. Häkkinen** and M. Manninen, "Ionization potential of Al\$_6\$ and Al\$_7\$ as a function of temperature", Europ. Phys. J D **9**, 179-182 (1999).
- (35) A. Rytkönen, **H. Häkkinen** and M. Manninen, "Melting and multipole deformation of sodium clusters", Europ. Phys. J D **9**, 451-454 (1999).
- (36) R. N. Barnett, C. L. Cleveland, **H. Häkkinen**, W. D. Luedtke, C. Yannouleas and U. Landman, "Structures and spectra of gold nanoclusters and quantum dots", Europ. Phys. J D **9**, 95-104 (1999).

- (37) E. Viitala, **H. Häkkinen**, M. Manninen and J. Timonen, "Spin Hamiltonians for small Ni clusters", Phys. Rev. B **61**, 8851 (2000).
- (38) **H. Häkkinen**, R. N. Barnett, A. G. Scherbakov and U. Landman, "Nanowire Gold Chains: Formation Mechanisms and Conductance", J. Phys. Chem B **104**, 9063-9066 (2000).
- (39) **H. Häkkinen** and U. Landman, "Gold clusters (Au_N , $2 \leq N \leq 10$) and their anions", Phys. Rev. B **62**, R2287-2290 (2000).
- (40) J. Akola, M. Manninen, **H. Häkkinen**, U. Landman, X. Li, and L.-S. Wang, "Aluminum Cluster Anions: Photoelectron Spectroscopy and Ab-initio Simulations", Phys. Rev. B **62**, 13216-13228 (2000).
- (41) M. Moseler, **H. Häkkinen**, R.N. Barnett and U. Landman, "Structure and Magnetism of Neutral and Anionic Pd Clusters", Phys. Rev. Lett. **86**, 2545-2548 (2001).
- (42) S. Abbet, U. Heiz, **H. Häkkinen** and U. Landman, "CO oxidation on a single Pd atom supported on magnesia", Phys. Rev. Lett. **86**, 5950-5953 (2001).
- (43) M. Moseler, **H. Häkkinen** and U. Landman, "Photoabsorption Spectra of Na_n^+ clusters: Thermal Line-Broadening Mechanisms", Phys. Rev. Lett. **87**, 053401 (2001).
- (44) **H. Häkkinen** and U. Landman, "Gas-phase catalytic oxidation of CO by Au_2^- ", J. Am. Chem. Soc. **123**, 9704-9705 (2001).
- (45) **H. Häkkinen**, M. Moseler and U. Landman, "Bonding in Cu, Ag, and Au clusters: Relativistic effects, trends, and surprises", Phys. Rev. Lett. **89**, 033401 (2002).
- (46) S. Abbet, A.M. Ferrari, L. Giordano, G. Pacchioni, **H. Häkkinen**, U. Landman, and U. Heiz, "Pd₁/MgO(100): A model system in Nanocatalysis", Surf. Sci. **514**, 249-255 (2002).
- (47) M. Moseler, **H. Häkkinen** and U. Landman, "Supported magnetic nanoclusters: Softlanding of Pd clusters on a MgO(100) surface", Phys. Rev. Lett. **89**, 176103 (2002).
- (48) **H. Häkkinen**, S. Abbet, A. Sanchez, U. Heiz and U. Landman, "Structural, electronic, and impurity-doping effects in nanoscale chemistry: Supported gold nanoclusters", Angew. Chem. Int. Ed. **42**, 1297 – 1300 (2003).
- (49) B. Yoon, **H. Häkkinen**, and U. Landman, "Interaction of O₂ with gold clusters: molecular and dissociative adsorption", J. Phys. Chem. A **107**, 4066 (2003).
- (50) L. D. Socaciu, J. Hagen, T. M. Bernhardt, L. Wöste, U. Heiz, **H. Häkkinen** and U. Landman, "Catalytic CO oxidation by free Au_2^- : Experiment and theory", J. Am. Chem. Soc. **125**, 10437 – 10445 (2003).
- (51) **H. Häkkinen**, B. Yoon, U. Landman, X. Li, H.-J. Zhai, and L.-S. Wang, "On the Electronic and Atomic Structures of Small Au_N^- ($N = 4-14$) Clusters: A Photoelectron Spectroscopy and Density-functional Study", J. Phys. Chem. A. **107**, 6168 – 6175 (2003).
- (52) M. Moseler, B. Huber, **H. Häkkinen**, U. Landman, G. Wrigge, M.A. Hoffmann, and B. v. Issendorff, "Thermal effects in the photoelectron spectra of Na_N^- clusters ($N=4-19$)", Phys. Rev. B. **68**, 165413 (2003).
- (53) K. Manninen, **H. Häkkinen**, and M. Manninen, "Electronic structure and thermal behavior of a magic Na_{59}^+ cluster", Phys. Rev. A **70**, 023203 (2004).

- (54) **H. Häkkinen**, M. Moseler, O. Kostko, N. Morgner, M. A. Hoffman, and B. v. Issendorff, "Symmetry and electronic structure of noble metal nanoparticles and the role of relativity", *Phys. Rev. Lett.* **93**, 093401-4 (2004).
- (55) R. N. Barnett, **H. Häkkinen**, A. G. Scherbakov and U. Landman, "Hydrogen Welding and Hydrogen Switches in a Mono-Atomic Gold Nanowire", *Nano Lett.* **4**, 1845 (2004).
- (56) B. Yoon, **H. Häkkinen**, U. Landman, A. Wörz, J.-M. Antonietti, S. Abbet, K. Judai, U. Heiz, "Charging Effects on Bonding and Catalyzed Oxidation of CO on Au₈ clusters on MgO", *Science* **307**, 403 (2005).
- (57) T. Santa-Nokki and **H. Häkkinen**, "Anomalous binding sequence of CO ligands to an anionic triplatinum carbonyl complex", *Chem. Phys. Lett.* **406**, 44 (2005).
- (58) K. Manninen, P. Pykkö and **H. Häkkinen**, "A small spherical liquid: DFT molecular dynamics study of WAu₁₂", *Phys. Chem. Chem. Phys.* **7**, 2208 - 2211 (2005).
- (59) K. Manninen, **H. Häkkinen**, and M. Manninen, "Ab initio simulation of Na₅₉⁺ and Na₉₃⁺", *Comput. Mater. Sci.* **35**, 158-162 (2005).
- (60) **H. Häkkinen** and M. Moseler, "55-atom clusters of silver and gold: Symmetry breaking by relativistic effects", *Comput. Mater. Sci.* **35**, 332-336 (2005).
- (61) B. Huber, **H. Häkkinen**, U. Landman and M. Moseler, "Oxidation of small gas phase Pd clusters: A density functional study", *Comput. Mater. Sci.* **35**, 371-374 (2005).
- (62) K. Manninen, T. Santa-Nokki, **H. Häkkinen**, and M. Manninen, "Magic clusters Na₅₇⁻ and Na₅₉⁺", *Eur. Phys. J D* **34**, 43-45 (2005).
- (63) M. Walter and **H. Häkkinen**, "Photoionization using Kohn-Sham wave functions", *Eur. Phys. J D* **33**, 393 (2005).
- (64) M. Walter and **H. Häkkinen**, "Optical absorption of magnesia-supported gold clusters and nanoscale catalysts: Effects due to the support, clusters, and adsorbants", *Phys. Rev. B* **72**, 205440 (2005).
- (65) **H. Häkkinen** and M. Walter, "Computational Spectroscopy of Supported Cluster nanocatalysts", Lecture Series on Computer and Computational Sciences, Vol. **4**, pp. 990-993 (2005).
- (66) B. Huber, P. Koskinen, H. Häkkinen, and **M. Moseler**, "Oxidation of Pd-clusters on magnesia leads to the ultimate limit of epitaxy with a catalytic function", *Nature Materials* **5**, 44 (2006).
- (67) P. Koskinen, **H. Häkkinen**, G. Seifert, S. Sanna, Th. Frauenheim and M. Moseler, "Density-functional based tight-binding study of small gold clusters", *New Journal of Physics* **8**, 9 (2006).
- (68) **H. Häkkinen**, M. Walter and H. Grönbeck, "Divide and Protect: Capping Gold Nanoclusters with Molecular Gold-Thiolate Rings", *J. Phys. Chem. B* **110**, 9927-9931 (2006).
- (69) M. Walter and **H. Häkkinen**, "A hollow tetrahedral cage of hexadecagold dianion provides a robust backbone for a sub-nanometer oxidation and reduction agent via endohedral doping", *Phys. Chem. Chem. Phys.* **8**, 5407 (2006).
- (70) P. Koskinen, **H. Häkkinen**, B. Huber, B.v. Issendorff, and M. Moseler, "Liquid-liquid phase coexistence in gold clusters: 2D or not 2D?", *Phys. Rev. Lett.* **98**, 015701 (2007).
- (71) B. Yoon, P. Koskinen, B. Huber, O. Kostko, B.v.Issendorff, **H. Häkkinen**, M. Moseler and U. Landman, "Size-dependent Structural Evolution and Chemical Reactivity of Gold Clusters",

ChemPhysChem. **8**, 157 (2007).

- (72) J. Akola and **H. Häkkinen**, "Ab initio study of the adsorption of gold atoms and clusters on graphite (0001) with defects", Phys. Rev. B **74**, 165404 (2006)
- (73) H. Grönbeck, M. Walter and **H. Häkkinen**, "Theoretical Characterization of Cyclic Thiolated Gold Clusters", J. Am. Chem. Soc. **128**, 10269 (2006).
- (74) H. Grönbeck and **H. Häkkinen**, "Polymerization at the Alkylthiolate-Au(111) Interface", J. Phys. B **111**, 3325 (2007).
- (75) K. Honkala and **H. Häkkinen**, "Au adsorption on regular and defected thin MgO(100) films supported by Mo", J. Phys. Chem. C **111**, 4319 (2007).
- (76) S. Tuukkanen, A. Kuzyk, V.P. Hytönen, **H. Häkkinen**, J.J. Toppari, E. Niskanen, M. Rinkiö and P. Törmä, "Trapping of 27 bp - 8kbp DNA and immobilization of thiol-modified DNA using dielectrophoresis", Nanotechnology **18**, 295204 (2007).
- (77) P. Frondelius, **H. Häkkinen**, K. Honkala, "Adsorption of gold clusters on metal-supported MgO: Correlation to electron affinity of gold", Phys. Rev. B **76**, 073406 (2007).
- (78) M. Walter, P. Frondelius, K. Honkala, **H. Häkkinen**, "Electronic structure of MgO-supported Au clusters: Quantum dots probed by STM", Phys. Rev. Lett. **99**, 096102 (2007)
- (79) M. Walter, **H. Häkkinen**, J. Stanzel, M. Neeb and W. Eberhardt, "Symmetry induced long-lived excited state in Au₆", Phys. Rev. B **76**, 155422 (2007).
- (80) P. Frondelius, **H. Häkkinen**, K. Honkala, "Adsorption of small Au clusters on MgO and MgO/Mo: the role of oxygen vacancies and the Mo-support", New Journal of Physics **9**, 339 (2007).
- (81) S. Malola, H. Häkkinen and P. Koskinen, "Raman intensity of single-walled carbon nanotubes with vacancies", Phys. Rev. B **77**, 155412 (2008)
- (82) M. Walter, J. Akola, O. Lopez-Acevedo, P. D. Jadzinsky, G. Calero, C. J. Ackerson, R. L. Whetten, H. Grönbeck, **H. Häkkinen**, "A unified view of ligand-protected gold clusters as superatom complexes", Proc. Natl. Acad. Sci. USA **105**, 9157 (2008)
- (83) J. Akola, M. Walter, R.L. Whetten, H. Häkkinen and H. Grönbeck, "On the structure of thiolate-protected Au₂₅", J. Am. Chem. Soc. **130**, 3756-3757 (2008).
- (84) P. Koskinen, S. Malola and **H. Häkkinen**, "Self-passivating reconstructions of graphene edges", Phys. Rev. Lett. **101**, 115502 (2008).
- (85) M. Walter, H. **Häkkinen**, L. Lehtovaara, M. Puska, J. Enkovaara, C. Rostgaard and J.J. Mortensen, "Time-dependent density-functional theory in the projector augmented-wave method", J. Chem. Phys. **128**, 244101 (2008)
- (86) P. Frondelius, A. Hellman, K. Honkala, **H. Häkkinen** and H. Grönbeck, "Charging of atoms, clusters and molecules on metal supported oxides: a general and long-ranged phenomenon", Phys. Rev. B **78**, 085426 (2008).
- (87) H. Grönbeck, **H. Häkkinen** and R.L. Whetten, "Gold-thiolate complexes form a unique c(4x2) structure on Au(111)", J. Phys. Chem. C **112**, 15940 (2008).
- (88) M. Walter and **H. Häkkinen**, "Photoelectron spectra from first principles: From many-body to single-particle picture", New J. Phys. **10**, 043018 (2008)

- (89) S. Malola, **H. Häkkinen** and P. Koskinen, "Effects of Bending on Raman-active Vibration Modes of Carbon Nanotubes", *Phys. Rev. B* **78**, 153409 (2008).
- (90) **H. Häkkinen**, "Atomic and electronic structure of gold clusters: understanding flakes, cages and superatoms from simple concepts", *Chem. Soc. Rev.* **37**, 1847 (2008)
- (91) S. Malola, **H. Häkkinen**, P. Koskinen, "Comparison of Raman spectra and vibrational density of states between graphene nanoribbons with different edges", *Eur. Phys. J. D* **52**, 71 (2009)
- (92) O. Lopez-Acevedo, D. Koudela, H. **Häkkinen**, "Conductance through atomic point contacts between fcc(100) electrodes of gold", *Eur. Phys. J. B* **66**, 497 (2008).
- (93) O. Lopez-Acevedo, J. Akola, R.L. Whetten, H. Grönbeck, **H. Häkkinen**, "Structure and Bonding in the Ubiquitous Icosahedral Metallic Gold Cluster Au₁₄₄(SR)₆₀", *J. Phys. Chem. C (Letter)* **113**, 5035 (2009) (cover article of issue 13, April 2, 2009).
- (94) S. Malola, **H. Häkkinen** and P. Koskinen, "Gold in graphene: in-plane adsorption and diffusion", *Appl. Phys. Lett.* **94**, 043106 (2009)
- (95) D. Koudela, A.-M. Uimonen and **H. Häkkinen**, "Conductance through analytic constrictions", *Eur. Phys. J. B* **68**, 111 (2009)
- (96) X. Lin, N. Nilius, H.-J. Freund, M. Walter, P. Frondelius, K. Honkala, **H. Häkkinen**, "Quantum well states in two-dimensional gold clusters on MgO thin films", *Phys. Rev. Lett.* **102**, 206801 (2009).
- (97) K. Kacprzak, J. Akola and **H. Häkkinen**, "First-principles simulations of hydrogen peroxide formation catalyzed by small neutral gold clusters", *Phys. Chem. Chem. Phys.* **11**, 6359 (2009).
- (98) K. Kacprzak, L. Lehtovaara, J. Akola, O. Lopez-Acevedo and **H. Häkkinen**, "A density functional investigation of thiolate-protected bimetal PdAu₂₄(SR)_{18(z)} clusters: Doping the superatom complex", *Phys. Chem. Chem. Phys.* **11**, 7123 (2009).
- (99) P. Koskinen, S. Malola and **H. Häkkinen**, "Evidence for Graphene Edges Beyond Zigzag and Armchair", *Phys. Rev. B* **80**, 073401 (2009).
- (100) O. Lopez-Acevedo, J. Rintala, S. Virtanen, C. Femoni, C. Tiozzo, H. Grönbeck, M. Pettersson and **H. Häkkinen**, "Characterization of Iron-carbonyl-protected Gold Clusters", *J. Am. Chem. Soc.* **131**, 12573 (2009).
- (101) P. Frondelius, **H. Häkkinen** and K. Honkala, "Adsorption and activation of O₂ at Au chains on MgO/Mo thin films", *Phys. Chem. Chem. Phys.* **12**, 1483 (2010).
- (102) O. Lopez-Acevedo, K.A.Kacprzak, J. Akola and **H. Häkkinen**, "Quantum size effects in ambient CO oxidation catalyzed by ligand-protected gold clusters", *Nature Chemistry* **2**, 329 (2010).
- (103) X. Lin, N. Nilius, M. Sterrer, P. Koskinen, **H. Häkkinen**, H-J. Freund, "Characterizing low-coordinated atoms at the periphery of MgO-supported Au islands", *Phys. Rev. B* **81**, 153406 (2010).
- (104) M. Strange, O. Lopez-Acevedo, **H. Häkkinen**, "Oligomeric gold-thiolate units define the properties of the molecular junction between gold and benzene dithiols", *J. Phys. Chem. Letters* **1**, 1528 (2010).
- (105) J.F. Parker, K.A. Kacprzak, O. Lopez-Acevedo, **H. Häkkinen**, R.W. Murray, "An experimental and density-functional theory analysis of serial introductions of electron-withdrawing ligands into the ligand shell of a thiolate-protected Au₂₅ nanoparticle", *J. Phys. Chem. C* **114**, 8276 (2010).

- (106) J. Akola, K.A. Kacprzak, O. Lopez-Acevedo, M. Walter, H. Grönbeck and **H. Häkkinen**, "Materials from thiolate-protected Au25 superatoms: Dimers and crystals", *J. Phys. Chem C* **114**, 15986 (2010).
- (107) S. Malola, **H. Häkkinen** and P. Koskinen, "Structural, chemical and dynamical trends in grain boundaries of graphene", *Phys. Rev. B* **81**, 165447 (2010). (*Editor's Suggestion to Read !*)
- (108) J. Enkovaara et al., Electronic structure calculations using GPAW: A real-space implementation of the projector-augmented wave method", *J. Phys. Condensed Matter* **22**, 253202 (2010).
- (109) O. Lopez-Acevedo, H. Tsunoyama, T. Tsukuda, **H. Häkkinen** and C.M. Aikens, "Chirality and electronic structure of the thiolate-protected Au38 nanocluster", *J. Am. Chem. Soc.* **132**, 8210 (2010).
- (110) K.A. Kacprzak, O. Lopez-Acevedo, **H. Häkkinen** and H. Grönbeck, "Theoretical characterization of cyclic thiolated copper, silver and gold clusters", *J. Phys. Chem. C* **114**, 13571 (2010).
- (111) P. Frondelius, **H. Häkkinen**, K. Honkala, "Ambient formation of gold(I) edge-oxide at flat gold nanoclusters on an ultra-thin MgO film", *Angew. Chemie Int. Ed.* **49**, 7913 (2010).
- (112) **H. Häkkinen** and R.L. Whetten, "Protected metallic clusters, quantum wells and metal-nanocrystal molecules", *J. Phys. Chem. C* **114**, 15877 (2010).
- (113) P.A. Clayborne, O. Lopez-Acevedo, R.L. Whetten, H. Grönbeck and **H. Häkkinen**, "Unified Interpretation of Cp(*) – protected Aluminum Clusters as Superatom Complexes", *Eur. J. Inorg. Chem.* **2011**, 2649 (2011).
- (114) O. Lopez-Acevedo and **H. Häkkinen**, "Derivatives of Au₂₅(SR)₁₈ cluster", *Eur. Phys. J. D* **63**, 311 (2011).
- (115) E. Hulkko, O. Lopez-Acevedo, J. Koivisto, Y. Levi-Kalisman, R.D. Kornberg, M. Pettersson and **H. Häkkinen**, "Electronic and vibrational signatures of the Au102(pMBA)44 cluster", *J. Am. Chem. Soc* **133**, 3752 (2011).
- (116) M. Strange, C. Rostgaard, **H. Häkkinen** and K.S. Thygesen, "First-principles many-body calculations of electronic conduction in thiol- and amine-linked molecules", *Phys. Rev. B* **83**, 115108 (2011). (Editor's Suggestion)
- (117) M. Walter, M. Moseler, R.L. Whetten and **H. Häkkinen**, "A 58-electron superatom-complex model for the magic phosphine-protected gold clusters (Schmid-gold, Nanogold) of 1.4-nm dimension", *Chemical Science* **2**, 1583 (2011).
- (118) L.J. Antila, M.J. Heikkilä, V. Mäkinen, N. Humalamäki, M. Laitinen, V. Linko, P. Jalkanen, J. Toppari, V. Aumanen, M. Kemell, P. Myllyperkiö, K. Honkala, **H. Häkkinen**, M. Leskelä and J.E.I. Korppi-Tommola, "ALD grown aluminum oxide submonolayers in dye-sensitized solar cells; The effect on interfacial electron transfer and performance", *J. Phys. Chem. C* **115**, 16720 (2011).
- (119) V. Mäkinen, K. Honkala and **H. Häkkinen**, "Atomic layer deposition of aluminum oxide on TiO₂ and its impact on N3 dye adsorption from first principles", *J. Phys. Chem. C* **115**, 9250 (2011).
- (120) O. Lopez-Acevedo, P.A. Clayborne and **H. Häkkinen**, "Electronic structure of Gold, Aluminum and Gallium superatom complexes", *Phys. Rev. B* **84**, 035434 (2011).
- (121) K. Salorinne, O. Lopez-Acevedo, E. Nauha, **H. Häkkinen** and M. Nissinen, "Solvent Driven Formation of Silver Embedded Resorcinarene Nanorods with Intracrystalline Enantiomeric Separation", *CrystEngComm.* **14**, 347 – 350 (2012).

- (122) P.A. Clayborne, O. Lopez-Acevedo, R.L. Whetten, H. Grönbeck and **H. Häkkinen**, "Evidence of superatomic electronic shells in ligand-stabilized aluminum clusters", *J. Chem. Phys.* **135**, 094701 (2011).
- (123) S. Malola and **H. Häkkinen**, "Electronic structure and bonding of icosahedral core-shell gold-silver nanoalloy clusters $\text{Au}_{144-x}\text{Ag}_x(\text{SR})_{60}$ ", *J. Phys. Chem. Lett.* **2**, 2316 (2011).
- (124) P.A. Clayborne and **H. Häkkinen**, "The Electronic Structure of $\text{Ge}_9[\text{Si}(\text{SiMe}_3)_3]_3$ -, A Superantiatom Complex", *Phys. Chem. Chem. Phys.* **14**, 9311 (2012).
- (125) E. Heikkilä, A.G. Gurtovenko, H. Martinez-Seara, **H. Häkkinen**, I. Vattulainen and J. Akola, "Atomistic Simulations of Functional $\text{Au}_{144}(\text{SR})_{60}$ Gold Nanoparticles in Aqueous Environment", *J. Phys. Chem. C* **116**, 9805 (2012).
- (126) L. Nykänen, **H. Häkkinen** and K. Honkala, "Computational study of linear carbon chains on gold and silver surfaces", *Carbon* **50**, 2752 (2012).
- (127) X. Chen, M. Strange and **H. Häkkinen**, "Non-magnetic and magnetic thiolate-protected Au_{25} superatoms on $\text{Cu}(111)$, $\text{Ag}(111)$ and $\text{Au}(111)$ surfaces", *Phys. Rev. B* **85**, 085422 (2012).
- (128) K. Salorinne, X. Chen, R.W. Troff, M. Nissinen and **H. Häkkinen**, "One-pot synthesis and characterization of subnanometer-size benzotriazolate protected copper clusters", *Nanoscale* **4**, 4095 (2012).
- (129) **H. Häkkinen**, "The gold-sulfur interface at the nanoscale", invited Review, *Nature Chemistry* **4**, 443 (2012).
- (130) C.L. Heinecke, T.W. Ni, S. Malola, V. Mäkinen, O.A. Wong, **H. Häkkinen** and C.J. Ackerson, "Structural and theoretical basis for ligand exchange on thiolate monolayer protected gold clusters", *J. Am. Chem. Soc.* **134**, 13316 (2012).
- (131) E. Guidez, V. Mäkinen, **H. Häkkinen** and C.M. Aikens, "Effects of Silver Doping on the Geometric and Electronic Structure and Optical Absorption Spectra of the $\text{Au}_{(25-n)}\text{Ag}_n(\text{SH})_{18-n}$ ($n = 1, 2, 4, 6, 8, 10, 12$) Bimetallic Nanoclusters", *J. Phys. Chem. C* **116**, 20617 (2012).
- (132) V. Mäkinen and **H. Häkkinen**, "Density functional molecular dynamics study of the $\text{Au}_{25}(\text{SR})_{18}$ -cluster", *Eur. Phys. J. D* **66**, 310 (2012).
- (133) X. Chen and **H. Häkkinen**, "Divide and protect: Passivating $\text{Cu}(111)$ by Cu-(benzotriazolate)2", *J. Phys. Chem. C* **116**, 22346 (2012).
- (134) J. Koivisto, S. Malola, A. Dass, **H. Häkkinen** and M. Pettersson, "Experimental and theoretical determination of the optical gap of the $\text{Au}_{144}(\text{SCH}_2\text{Ph})_{60}$ cluster and the $(\text{AuAg})_{144}(\text{SCH}_2\text{Ph})_{60}$ nanoalloys", *J. Phys. Chem. Lett.* **3**, 3076 (2012).
- (135) V. Mäkinen, P. Koskinen and **H. Häkkinen**, "Modelling thiolate-protected gold clusters with density-functional tight-binding", *Eur. Phys. J. D* **67**, 38 (2013).
- (136) S. Malola, L. Lehtovaara, S. Knoppe, K.-J. Hu, R. Palmer, T. Burgi and **H. Häkkinen**, "Au $40(\text{SR})_{24}$ Cluster as a Chiral Dimer of 8-Electron Superatoms: Structure and Optical Properties", *J. Am. Chem. Soc.* **134**, 19560 (2012).
- (137) J. Andersin, J. Nevalaita, K. Honkala and **H. Häkkinen**, "The redox chemistry of gold with high-valence doped CaO", *Angew. Chemie Int. Ed.* **52**, 1424 (2012).

- (138) K. Salorinne, T. Lahtinen, J. Koivisto, E. Kalenius, M. Nissinen, M. Pettersson, **H. Häkkinen**, "Non-destructive size determination of thiol-stabilized gold nanoclusters in solution by DOSY NMR spectroscopy", *Anal. Chem.* **85**, 3489 (2013).
- (139) K. Helttunen, L. Lehtovaara, **H. Häkkinen** and M. Nissinen, "Crystal structures and density functional theory calculations of o- and p-nitroaniline ligands: combined effect of hydrogen bonding and aromatic interactions on dimerization energy", *Cryst. Growth Des.* **13**, 3603 (2013).
- (140) H. Yang, Y. Wang, J. Lei, L. Shi, X. Wu, V. Mäkinen, S. Lin, Z. Tang, J. He, **H. Häkkinen**, L. Zheng and N. Zheng, "Ligand-stabilized Au₁₃Cux (x=2,4,8) bimetallic nanoclusters: Ligand-engineering to control the exposure of metal sites", *J. Am. Chem. Soc.* **135**, 9568 (2013).
- (141) X. Chen and **H. Häkkinen**, "Protected but accessible: Oxygen activation by a calixarene-stabilized undecagold cluster", *J. Am. Chem. Soc.* **135**, 12944-12947 (2013).
- (142) C. Stiehler, Y. Pan, W.-D. Schneider, P. Koskinen, **H. Häkkinen**, N. Nilius and H.-J. Freund, "Electron quantization in arbitrarily shaped gold islands on MgO thin films", *Phys. Rev. B* **88**, 115415 (2013).
- (143) H. Yang, Y. Wang, H. Huang, L. Gell, L. Lehtovaara, S. Malola, **H. Häkkinen** and N. Zheng, "All-thiol-stabilized Ag₄₄ and Au₁₂Ag₃₂ nanoparticles with single-crystal structures", *Nature Communications* **4**, 2422 (2013).
- (144) A. Mathew, G. Natarajan, L. Lehtovaara, **H. Häkkinen**, R.M. Kumar, V. Subramanian, A. Jaleel and T. Pradeep, "Supramolecular functionalization and concomitant enhancement in properties of Au₂₅ clusters", *ACS Nano* **8**, 139-152 (2014).
- (145) J. Q. Goh, S. Malola, **H. Häkkinen** and J. Akola, "The role of central gold atom in ligand-protected bi-icosahedral Au₂₄ and Au₂₅ clusters", *J. Phys. Chem. C* **117**, 22079 (2013).
- (146) S. Knoppe, S. Malola, L. Lehtovaara, T. Buergi and **H. Häkkinen**, "Electronic structure and optical properties of the thiolate-protected Au₂₈(SMe)₂₀ cluster", *J. Phys. Chem. A* **117**, 10526 (2013).
- (147) C.G. Rocha, P.A. Clayborne, P. Koskinen and **H. Häkkinen**, "Optical and electronic properties of graphene nanoribbons upon adsorption of ligand-protected aluminum clusters", *PCCP* **16**, 3558 (2014).
- (148) I. Chakraborty, W. Kurashige, K. Kanemura, L. Gell, **H. Häkkinen**, Y. Negishi, T. Pradeep, "Ag₄₄(SeR)₃₀: A highly stable selenolate protected silver cluster", *J. Phys. Chem. Lett.* **4**, 3351 (2013).
- (149) S. Malola, L. Lehtovaara, J. Enkovaara, **H. Häkkinen**, "Birth of the localized surface plasmon resonance in monolayer-protected gold nanoclusters", *ACS Nano* **7**, 10263 (2013).
- (150) V. Marjomäki, T. Lahtinen, M. Martikainen, J. Koivisto, S. Malola, K. Salorinne, M. Pettersson and **H. Häkkinen**, "Site-specific targeting of enterovirus capsid by functionalized monodisperse gold nanoclusters", *Proc. Natl. Acad. Sci. USA* **111**, 1277-1281 (2014).
- (151) J. Hassinen, P. Pulkkinen, E. Kalenius, T. Pradeep, H. Tenhu, **H. Häkkinen**, R.H.A. Ras "Au₂₅ clusters with calix[4]arene functionalities", *J. Phys. Chem. Lett.* **5**, 585-589 (2014).
- (152) D. Crasto, S. Malola, G. Brosovsky, A. Dass and **H. Häkkinen**, "Single Crystal XRD Structure and Theoretical Analysis of the Chiral Au₃₀S(S-t-Bu)₁₈ Cluster", *J. Am. Chem. Soc.* **136**, 5000 (2014).
- (153) J. Koivisto, K. Salorinne, S. Mustalahti, T. Lahtinen, S. Malola, **H. Häkkinen**, M. Pettersson "Vibrational perturbations and ligand-layer coupling in a single crystal of Au₁₄₄(SC₂H₄Ph)₆₀", *J. Phys. Chem. Lett.* **5**, 387 (2014).

- (154) L. Gell, L. Lehtovaara and **H. Häkkinen**, "Superatomic S₂ Silver Clusters Stabilized by Thiolate – Phosphine Monolayer: Insight into Electronic and Optical Properties of Ag₁₄(SC₆H₃F₂)₁₂(PPh₃)₈ and Ag₁₆(SC₆H₃F₂)₁₄(DPPE)₄", *J. Phys. Chem. A* **118**, 8351–8355 (2014).
- (155) S. Malola, L. Lehtovaara and **H. Häkkinen**, "A DFT study of linear gold-thiolate superclusters absorbing in the therapeutic NIR window", *J. Phys. Chem. Lett.* **5**, 1329 (2014).
- (156) S. Knoppe, O.A. Wong, S. Malola, **H. Häkkinen**, T. Buergi, T. Verbiest and C.J. Ackerson, "Chiral phase transfer and enantioenrichment of thiolate-protected Au₁₀₂ clusters", *J. Am. Chem. Soc.* **136**, 4129 (2014).
- (157) H. Yang, Y. Wang, J. Yan, X. Chen, X. Zhang, **H. Häkkinen** and N. Zheng, "Structural evolution of atomically precise thiolated bimetallic Au_{12+n}Cu₃₂(SR)_{30+n}⁴⁻ (n=0,2,4,6) clusters", *J. Am. Chem. Soc.* **136**, 7197 (2014)
- (158) E. Heikkilä, H. Martinez-Seara, A.A. Gurtovenko, M. Javanainen, **H. Häkkinen**, I. Vattulainen and J. Akola, "Cationic Au nanoparticle binding with plasma membrane-like lipid bilayers: Potential mechanism for spontaneous permeation to cells revealed by atomistic simulations", *J. Phys. Chem. C* **118**, 11131 (2014).
- (159) K. Salorinne, T. Lahtinen, S. Malola, J. Koivisto and **H. Häkkinen**, "Solvation chemistry of water-soluble thiol-protected gold nanoclusters Au₁₀₂ and Au₁₄₄ from DOSY NMR spectroscopy and DFT calculations", *Nanoscale* **6**, 7823 (2014).
- (160) S. Knoppe, L. Lehtovaara and **H. Häkkinen**, "Electronic Structure and Optical Properties of the Intrinsically Chiral 16-Electron Superatom Complex (Au₂₀(PP₃)₄)⁴⁺", *J. Phys. Chem. A* **118**, 4214 (2014).
- (161) S. Mustalahti, P. Myllyperkiö, T. Lahtinen, K. Salorinne, S. Malola, J. Koivisto, **H. Häkkinen**, M. Pettersson "Ultrafast Electronic Relaxation and Vibrational Cooling Dynamics of Au₁₄₄(SC₂H₄Ph)₆₀ Nanocluster Probed by Transient Mid-IR Spectroscopy", *J. Phys. Chem. C* **118**, 18233 (2014).
- (162) M. Azubel, J. Koivisto, S. Malola, D. Bushnell, G.L. Hura, A.L. Koh, H. Tsunoyama, T. Tsukuda, M. Pettersson, **H. Häkkinen** and R.D. Kornberg, "Electron microscopy of gold nanoparticles at atomic resolution", *Science* **345**, 909 (2014).
- (163) S. Malola, L. Lehtovaara and **H. Häkkinen**, "A TDDFT analysis of optical properties of thiol monolayer-protected Au₁₄₄(SR)₆₀ and Au₈₄Ag₆₀(SR)₆₀ clusters", *J. Phys. Chem. C* **118**, 20002–20008 (2014).
- (164) W.S. Compel, O.A. Wong, X. Chen, C. Yi, **H. Häkkinen**, K. Knappenberger and C. Ackerson, "Dynamic diglyme-mediated self-assembly of gold nanoparticles", *ACS Nano* **9**, 11690 (2015).
- (165) K. Salorinne, T. Lahtinen, V. Marjomäki and **H. Häkkinen**, "Polymorphic and solvate structures of ethyl ester and carboxylic acid derivatives of WIN 61893 analogue and their stability in solution", *CrystEngComm.* **16**, 9001–9009 (2014).
- (166) A. Baksi, M.S. Bootharaju X. Chen, **H. Häkkinen** and T. Pradeep , "Ag₁₁(SG)₇: A new cluster identified by mass spectrometry and optical spectroscopy", *J. Phys. Chem. C* **118**, 21722 (2014).
- (167) S. Mustalahti, P. Myllyperkiö, S. Malola, T. Lahtinen, K. Salorinne, J. Koivisto, **H. Häkkinen** and M. Pettersson, "Molecule-like photodynamics of Au₁₀₂(pMBA)₄₄ nanocluster", *ACS Nano* **9**, 2328 (2015).
- (168) L. Gell and **H. Häkkinen**, "A theoretical analysis of the M₁₂Ag₃₂(SR)₃₀⁴⁻ and X@M₁₂Ag₃₂(SR)₃₀⁴⁻ nanoclusters (M = Au, Ag; X = H, Mn)", *J. Phys. Chem. C* **119**, 10943 (2015).

- (169) J.Q. Goh, S. Malola, **H. Häkkinen** and J. Akola, "Silver Sulfide Nanoclusters and the Superatom Model", *J. Phys. Chem. C* **119**, 1583 (2015).
- (170) M. Hartman, **H. Häkkinen**, J. Millstone and D. Lambrecht, "Impacts of copper position on electronic structure of $\text{Au}_{25-x}\text{Cu}_x(\text{SH})_{18}^-$ nanoclusters", *J. Phys. Chem. C* **119**, 8290 (2015).
- (171) S. Malola, M. Hartman and **H. Häkkinen**, "Copper induces a core plasmon in intermetallic $\text{Au}_{(144,145)-x}\text{Cu}_x(\text{SR})_{60}$ nanoclusters", *J. Phys. Chem. Lett.* **6**, 515 (2015).
- (172) Y. Negishi, T. Nakazaki, S. Malola, S. Takano, Y. Niihori, W. Kurashige, S. Yamazoe, T. Tsukuda and **H. Häkkinen**, "A critical size for emergence of nonbulk electronic and geometric structures in dodecanethiolate-protected Au clusters", *J. Am. Chem. Soc.* **137**, 1206 (2015).
- (173) M.A. Tofanelli, S. Malola, T. Ni, K. Salorinne, B. Newell, B. Phillips, **H. Häkkinen** and C.J. Ackerson, "Jahn-Teller effects in $\text{Au}_{25}(\text{SR})_{18}$ ", *Chemical Science* **7**, 1882-1890 (2015).
- (174) T.-R. Tero, K. Salorinne, S. Malola, **H. Häkkinen** and M. Nissinen, "Solid state halogen bonded networks vs. dynamic assemblies in solution: Explaining N...X interactions of multivalent building blocks", *CrystEngCOmm* **17**, 8231 (2015).
- (175) E. Pohjolainen, **H. Häkkinen** and A. Clayborne, "The role of the anchor atom in the ligand of the monolayer-protected Au_{25}^- nanocluster", *J. Chem. C* **119**, 9587 (2015).
- (176) F. Calaza, C. Stiehler, Y. Fujimori, M. Sterrer, S. Beeg, M. Ruiz-Oses, N. Nilius, M. Heyde, T. Parviainen, K. Honkala, **H. Häkkinen** and H.-J. Freund "Carbon Dioxide Activation and Reaction Induced by Electron-Transfer at an Oxide-Metal Interface", *Angew. Chemie Int. Ed.* **54**, 12484 (2015).
- (177) M. Martikainen, K. Salorinne, T. Lahtinen, S. Malola, P. Permi, **H. Häkkinen** and V. Marjomäki, "Hydrophobic pocket targeting probe for enteroviruses", *Nanoscale* **7**, 17457 (2015).
- (178) S. Knoppe, **H. Häkkinen** and T. Verbiest, "Nonlinear Optical Properties of Thiolate-Protected Gold Clusters: A Theoretical Survey of the First Hyperpolarizabilities", *J. Phys. Chem. C* **119**, 27676 (2015).
- (179) S. Mustalahti, P. Myllyperkiö, T. Lahtinen, S. Malola, K. Salorinne, T.-R. Tero, J. Koivisto, **H. Häkkinen** and M. Pettersson, "Photodynamics of a molecular water-soluble nanocluster identified as (about) $\text{Au}_{130}(\text{pMBA})_{50}$ ", *J. Phys. Chem. C* **119**, 20224 (2015).
- (180) H. Yang, Y. Wang, X. Chen, X. Zhao, L. Gu, H. Huang, J. Yan, C. Xu, G. Li, J. Wu, A.J. Edwards, B. Dittrich, Z. Tang, D. Wang, L. Lehtovaara, **H. Häkkinen** and N.F. Zheng, "Plasmonic twinned silver nanoparticles with molecular precision", *Nature Comm.* **7**, 12809 (2016).
- (181) J. Yan, H. Su, H. Yang, S. Malola, S. Lin, **H. Häkkinen** and N.F. Zheng, "Total structure and electronic structure analysis of doped thiolated silver ($\text{MAg}_{24}(\text{SR})_{18}2-$ (M = Pd, Pt) clusters", *J. Am. Chem. Soc.* **137**, 11880 (2015).
- (182) B. Zhang, S. Kaziz, H.H. Li, D. Wodka, S. Malola, O. Safanova, M. Nachtegaal, C. Mazet, I. Dolamic, J. Liorca, E. Kalenius, L.M.L. Daku, **H. Häkkinen**, T. Burgi and N. Barrabes, "Pd₂Au₃₆(SR)₂₄ cluster: structural studies", *Nanoscale* **7**, 17012 (2015).
- (183) J. Nevalaita, **H. Häkkinen** and K. Honkala, "Dissociative adsorption of water on Au/MgO/Ag(001) from first principles calculations", *Surf. Sci.* **640**, 10 (2015).
- (184) Y. Wang, H. Su, C. Xu, G. Li, L. Gell, S. Lin, Z. Tang, **H. Häkkinen** and N.F. Zheng, "An intermetallic $\text{Au}_{24}\text{Ag}_{20}$ Superatom Nanocluster Stabilized by Labile Ligands", *J. Am. Chem. Soc.* **137**,

4324 (2015).

- (185) K. Salorinne, S. Malola, O.A. Wong, C.D. Rithner, X. Chen, C.J. Ackerson and **H. Häkkinen**, "Conformation and dynamics of the ligand shell of a water-soluble Au102 nanoparticle", *Nature Comm.* **7**, 10401 (2016).
- (186) N. van Steerteghem, S. van Cleuvenbergen, S. Deckers, C. Kumara, A. Dass, **H. Häkkinen**, K. Clays, T. Verbiest and S. Knoppe, "Symmetry breaking in ligand-protected gold clusters probed by nonlinear optics", *Nanoscale* **8**, 12123-12127 (2016).
- (187) Y. Wang, X.K. Wan, L. Ren, H.F. Su, G. Li, S. Malola, S.C. Lin, Z. Tang, **H. Häkkinen**, B. Teo, Q.M. Wang and N.F. Zheng, "Atomically Precise Alkynyl-Protected Metal Nanoclusters as a Model Catalyst: Observation of Promoting Effect of Surface Ligands on Catalysis by Metal Nanoparticles", *J. Am. Chem. Soc.* **138**, 3278 (2016).
- (188) E. Pohjolainen, X. Chen, S. Malola, G. Groenhof and **H. Häkkinen**, "A Unified AMBER-Compatible Molecular Mechanics Force Field for Thiolate Protected Gold Nanoclusters", *J. Chem. Theory Comp.* **12**, 1342 (2016).
- (189) J. Koivisto, X. Chen, S. Donnini, T. Lahtinen, **H. Häkkinen**, G. Groenhof and M. Pettersson, "Acid-base properties and surface charge distribution of the water-soluble Au102(pMBA)44 nanocluster", *J. Phys. Chem. C* **120**, 10041 (2016).
- (190) M. Hartmann, J.E. Millstone and **H. Häkkinen**, "Surface chemistry controls magnetism in cobalt nanoclusters", *J. Phys. Chem. C* **120**, 20822-20827 (2016).
- (191) J. Nevalaita, **H. Häkkinen** and K. Honkala, "Gold assisted oxygen dissociation on a Molybdenum-doped CaO(001) surface", *Catal. Sci. Technol.* **6**, 6784-6793 (2016).
- (192) M.J. Alhilaly, M. S. Bootharaju, C.P. Joshi, T.M. Besong, A.H. Emwas, R. Juarez-Mosqueda, S. Kaappa, S. Malola, K. Adil, A. Shkurenko, **H. Häkkinen**, M. Eddaoudi and O.M. Bakr, "(Ag₆₇(SPhMe₂)₃₂(PPh₃)₈)³⁺: Synthesis, total structure, and optical properties of a large box-shaped silver nanocluster", *J. Am. Chem. Soc.* **138**, 14727-14732 (2016).
- (193) T. Lahtinen, E. Hulkko, K. Sokolowska, T-R. Tero, V. Saarnio, J. Lindgren, M. Pettersson, **H. Häkkinen** and L. Lehtovaara, "Covalently linked multimers of gold nanoclusters Au102(pMBA)44 and Au~250)(pMBA)_n", *Nanoscale* **8**, 18665-18674 (2016).
- (194) **H. Häkkinen**, "Electronic shell structures in bare and protected metal nanoclusters", *Advances in Physics X* **1**, 467-491 (2016).
- (195) J. Yan, H. Su, H. Yang, C. Hu, S. Malola, S. Lin, B.K. Teo, **H. Häkkinen** and N.F. Zheng, "Asymmetric Synthesis of Chiral Bimetallic (Ag₂₈Cu₁₂(SR)₂₄)₍₄₋₎ Nanoclusters via Ion Pairing", *J. Am. Chem. Soc.* **138**, 12751-12754 (2016).
- (196) C. Stiehler, N. Nilius, J. Nevalaita, K. Honkala and **H. Häkkinen**, "Gold/Isophorone Interaction Driven by Keto/Enol Tautomerization", *J. Phys. Chem. C* **120**, 21962-21966 (2016).
- (197) R. Juarez-Mosqueda, S. Kaappa, S. Malola and **H. Häkkinen**, "Analysis of the electronic structure of non-spherical ligand-protected metal nanoclusters: The case of a box-like Ag₆₇", *J. Phys. Chem. C* **121**, 10698-10705 (2017).
- (198) Y. Wang, H. Su, L. Ren, S. Malola, S. Lin, B.K. Teo, **H. Häkkinen**, and Nanfeng Zheng, "Site preference in multi-metallic nanoclusters: Incorporation of alkali-metals ions or copper atoms into alkynyl-

protected body-centered-cubic ($\text{Au}_7\text{Ag}_8(\text{CtBu})_{12}$)⁺ cluster", *Angew. Chemie Int. Ed.* **55**, 15152-15156 (2016).

(199) H. Yang, J. Yan, Y. Wang, H.-F. Su, L. Gell, X. Zhao, C. Xu, **H. Häkkinen**, B.K. Teo, N. Zheng, "Embryonic Growth of Face-Center-Cubic Silver Nanoclusters Shaped in Nearly Perfect Half-Cubes and Cubes", *J. Am. Chem. Soc.* **139**, 31-34 (2017).

(200) Nonappa, T. Lahtinen, J.S. Haataja, T.R. Tero, **H. Häkkinen**, and O.Ikkala, "Template-free supracolloidal self-assembly of atomically precise gold nanoclusters: From 2D colloidal crystals to spherical capsids", *Angew. Chemie Int. Ed.* **55**, 16035-16038 (2017).

(201) Nonappa, J.S. Haataja, J.V. Timonen, S. Malola, P. Engelhardt, N. Houbenov, M. Lahtinen, H. **Häkkinen**, and O.Ikkala, "Reversible supracolloidal self-assembly of cobalt nanoparticles to hollow capsids and their superstructures", *Angew. Chemie Int. Ed.* **56**, 6473 (2017).

(202) J. Nevalaita, **H. Häkkinen** and K. Honkala, "Isophorone on Au/MgO/Ag(001): Physisorption with electrostatic site selection", *J. Phys. Chem. C* **121**, 10824 (2017).

(203) M.S. Kuklin, A. S. Bazhenov, K. Honkala, S. Tosoni, G. Pacchioni, and **H. Häkkinen**, "Structure and dynamics of CaO films: a computational study of an effect of external static electric field", *Phys. Rev. B* **95**, 165423 (2017).

(204) R. Juarez-Mosqueda, S. Kaappa, S. Malola and **H. Häkkinen**, "Stability, electronic structure, and optical properties of protected gold-doped silver Ag_{29-x}Au_x (x=0-5) nanoclusters", *Phys. Chem. Chem. Phys.* **21**, 13868 (2017).

(205) J. Liu, N. Jian, I. Ornelas, A.J. Pattison, T. Lahtinen, K. Salorinne, **H. Häkkinen** and R.E. Palmer, "Exploring the atomic structures of 1.8 nm monolayer-protected gold clusters with aberration-corrected STEM", *Ultramicroscopy* **176**, 146-150 (2017).

(206) E. Pohjolainen, S. Malola, G. Groenhof and **H. Häkkinen**, "Exploring strategies for labeling viruses with gold nanoclusters through non-equilibrium molecular dynamics simulations", *Bioconjugate Chem.* **28**, 2327-2339 (2017).

(207) L. Ren, P. Yuan, H. Su, S. Malola, S. Lin, Z. Tang, B.K. Teo, **H. Häkkinen**, L. Zheng and N.F. Zheng, "Bulky surface ligands promote surface reactivities of ($\text{Ag}_{141}\text{X}_{12}(\text{S-Adm})_{40}$)³⁺ (X=Cl, Br, I) nanoclusters: Models for multiple-twinned nanoparticles", *J. Am. Chem. Soc.* **139**, 13288-13291 (2017).

(208) E. Selenius, S. Malola and **H. Häkkinen**, "Analysis of localized surface plasmon resonances in spherical jellium clusters and their assemblies", *J. Phys. Chem. C* **121**, 27036-27052 (2017).

(209) T.R. Tero, S. Malola, B. Koncz, E. Pohjolainen, S. Lautala, S. Mustalahti, P. Permi, G. Groenhof, M. Pettersson and **H. Häkkinen**, "Dynamic stabilization of the ligand-metal interface in atomically precise gold nanoclusters Au₆₈ and Au₁₄₄ protected by meta-mercaptopbenzoic acid", *ACS Nano* **11**, 11872-11879 (2017).

(210) M. C. Stark, M. A. Baikoghli, T. Lahtinen, S. Malola, L. Xing, M. Nguyen, M. Nguyen, A. Sikaroudi, V. Marjomäki, **H. Häkkinen** and R. H. Cheng, "Structural characterization of site-modulated nanocapsid with monodispersed gold clusters", *Scientific Reports* **7**, 17048 (2017).

(211) L.S. Slaughter, K.M. Cheung, S. Kaappa, H.H. Cao, Q. Yang, T.D. Young, A. C. Serino, S. Malola, J.M. Olson, S. Link, **H. Häkkinen**, A.M. Andrews and P.S. Weiss, "Patterning Supported Gold Monolayers via Chemical Lift-Off Lithography", *Beilstein Journal of Nanotechnology* **8**, 2648-2661 (2017).

- (212) S. Kenzler, C. Schrenk, A.R. Frojd, **H. Häkkinen**, A.Z. Clayborne and A. Schnepf, “Au70S20(PPh₃)₁₂: An intermediate sized metalloid gold cluster stabilized by the Au₄S₄ ring motif and Au-PPh₃ groups”, *Chem. Comm.* **54**, 248-251 (2018).
- (213) **H. Häkkinen** and C. Aikens, ”Connections between Theory and Experiment for Gold and Silver Nanoclusters“, *Annual Review of Physical Chemistry*, Vol. **69**, 205-229 (2018).
- (214) M. J. Hartmann, J.E. Millstone and **H. Häkkinen**, “Ligand Mediated Evolution of Size Dependent Magnetism in Cobalt Nanoclusters”, *Phys. Chem. Chem. Phys.* **20**, 4563 – 4570 (2018).
- (215) G. Deng, S. Malola, J. Yan, Y.Z. Han, P. Yuan, C. Zhao, X, Yuan, S. Lin, Z. Tang, B.K. Teo, **H. Häkkinen** and N. Zheng, “From Symmetry Breaking to Unraveling Chirality of Metal Nanoclusters”, *Angew. Chem. Int. Ed.* **57**, 3421-3425 (2018).
- (216) S. Knoppe, **H. Häkkinen**, T. Verbiest and K. Clays, “ The Role of Donor and Acceptor Substituents on the Nonlinear Optical Properties of Gold Nanoclusters, *J. Phys. Chem.* **122**, 4019-4028 (2018).
- (217) A. Chakraborty, A.C. Fernandez, A. Som, B. Mondal, Nonappa, G. Natarajan, G. Paramasivan, T. Lahtinen, **H. Häkkinen** and T. Pradeep, ”Atomically Precise Nanocluster Assemblies Encapsulating Plasmonic Gold Nanorods”, *Angew. Chemie Int. Ed.* **57**, 6522-6526 (2018).
- (218) J. Yan, J. Zhang, X. Chen, S. Malola, B. Zhou, E. Selenius, X. Zhang, P. Yuan, G. Deng, K. Liu, H. Su, B.K. Teo, **H. Häkkinen**, L. Zheng and N. Zheng, “Thiol-Stabilized Atomically Precise, Superatomic Silver Nanoparticles for Catalyzing Cycloisomerization of Alkynyl Amines”, *National Science Review* **5**, 694-702 (2018).
- (219) Q. Zhou, S. Kaappa, S. Malola, H. Lu, D. Guan, Y. Li, H. Wang, Z. Xie, Z. Ma, **H. Häkkinen**, N. Zheng, X. Yang and L. Zheng, “Real-Space Imaging with Pattern Recognition of a Ligand-Protected Ag₃₇₄ Nanocluster at Sub-Molecular Resolution”, *Nature Comm.* **9**, 2948 (2018).
- (220) J. Yan, S. Malola, C. Hu, P. Yuan, G. Deng, H. Yang, B. Dittrich, B.K. Teo, **H. Häkkinen** and N. Zheng, “Co-Crystallization of Atomically Precise Metal Nanoparticles Driven by Magic Atomic and Electronic Shells“, *Nature Comm.* **9**, 3357 (2018).
- (221) M.S. Kuklin, K. Honkala and **H. Häkkinen**, ”A Computational Study of Adsorption of CO₂, SO₂ and H₂CO on Free-Sanding and Mo-Supported CaO Films”, *J. Phys. Chem. C* **123**, 7758-7765 (2019).
- (222) S. Kaappa, S. Malola and **H. Häkkinen**, "Point Group Symmetry Analysis of the Electronic Structure of Bare and Protected Metal Nanoclusters", *J. Phys. Chem. A* **122**, 8576-8584 (2018).
- (223) K. Sokolowska, S. Malola, M. Lahtinen, V. Saarnio, P. Permi, K. Koskinen, M. Jalasvuori, **H. Häkkinen**, L. Lehtovaara and T. Lahtinen, ”Towards Controlled Synthesis of Water-Soluble Gold Nanoclusters: Synthesis and Analysis”, *J. Phys. Chem C* **123**, 2602-2612 (2019).
- (224) M.R. Narouz, P.J. Unsworth, K. Salorinne, S. Takano, R. Tomihara, S. Kaappa, S. Malola, C.T. Dingh, J.D. Padmos, K. Ayoo, P.J. Garrett, M. Nambo, J. Hugh Horton, E.H. Sargent, **H. Häkkinen**, T. Tsukuda and C.M. Crudden, “N-Heterocyclic Carbene-Functionalized Magic Number Gold Nanoclusters”, *Nature Chem.* **11**, 419-425 (2019).
- (225) X. Yuan, X. Li, S. Malola, B.K. Teo, **H. Häkkinen**, L Zheng and N. Zheng, “Combinatorial Identification of Hydrides in a Ligated Ag₄₀ Nanocluster with Noncompact Metal Core”, *J. Am. Chem. Soc.* **141**, 11905-11911 (2019).
- (226) S. Malola and **H. Häkkinen**, “Chiral Inversion of Thiolate-Protected Gold Nanoclusters via Core Reconstruction without Breaking an Au-S Bond“, *J. Am. Chem. Soc.* **141**, 6006-6012 (2019).

- (227) R. Juarez-Mosqueda, S. Malola and **H. Häkkinen**, “Ab initio molecular dynamics studies of Au₃₈(SR)₂₄ isomers under heating”, *Eur. Phys. J D* **73**, 62 (2019).
- (228) C. Sun, N. Mammen, S. Kaappa, P. Yuan, G. Deng, C. Zhao, J. Yan, S. Malola, K. Honkala, **H. Häkkinen**, B.K. Teo and N. Zheng, “Atomically precise, thiolated copper-hydride nanoclusters as single-site hydrogenation catalysts for ketones in mild conditions”, *ACS Nano* **13**, 5975-5986 (2019).
- (229) M.S. Bootharaju, H. Chang, G. Deng, S. Malola, W. Baek, **H. Häkkinen**, N. Zheng and T. Hyeon, “Cd₁₂Ag₃₂(SePh)₃₆: Non-noble metal doped silver nanocluster”, *J. Am. Chem. Soc.* **141**, 8422-8425 (2019).
- (230) S. Malola and **H. Häkkinen**, ”Chiral footprint of the ligand layer in the all-alkynyl-protected gold nanocluster Au₁₄₄(CCPhF)₆₀”, *Chem. Comm.* **55**, 9460-9462 (2019).
- (231) S. Malola, S. Kaappa and **H. Häkkinen**, “The role of nanocrystal symmetry in the crossover region from molecular to metallic gold nanoparticles”, *J. Phys. Chem. C* **123**, 20655-20663 (2019).
- (232) S. Malola, P. Nieminen, A. Pihlajamäki, J. Hämäläinen, T. Kärkkäinen and **H. Häkkinen**, ”A method for structure prediction of metal-ligand interfaces of hybrid nanoparticles”, *Nature Comm.* **10**, 3973 (2019).
- (233) M.R. Narouz, S. Takano, P. A. Lummis, T. I. Levchenko, A. Nazemi, S. Kaappa, S. Malola, G. Yousefizadeh, L.A. Calhoun, K.G. Stamplecoskie, **H. Häkkinen**, T. Tsukuda, C.M. Crudden, ”Robust, highly luminescent Au₁₃ superatoms protected by N-heterocyclic carbenes”, *J. Am. Chem. Soc.* **141**, 14997-15002 (2019).
- (234) H. Shen, G. Deng, S. Kaappa, T. Tan, Y.Z. Han, S. Malola, S.C. Lin, B.K. Teo, **H. Häkkinen**, N. Zheng, ”Highly robust but surface-active: N-heterocyclic carbene-stabilized Au₂₅ nanocluster”, *Angew. Chemie Int. Ed.* (2019). DOI: 10.1002/anie.201908983
- (235) A. Longo, E.J.J. de Boed, N. Mammen, M. van der Linden, K. Honkala, **H. Häkkinen**, P.E. deJongh and B. Donoeva, ”Towards atomically precise supported catalysts from monolayer-protected clusters: The critical role of the support”, *Chem – Eur J* (accepted) <http://dx.doi.org/10.1002/chem.202000637>
- (236) Y. Tasaka, K. Nakamura, S. Malola, K. Hirata, K. Kim, K. Koyasu, **H. Häkkinen** and T. Tsukuda, ”Electron binding in a superatom with a repulsive Coulomb barrier: The case of Ag₄₄(SR)₃₀ 4- in gas phase”, *J. Phys. Chem. Lett.* <https://pubs.acs.org/doi/pdf/10.1021/acs.jpclett.0c00786>
- (237) P. Yuan, R. Zhang, E. Selenius, P. Ruan, Y. Yao, Y. Zhou, S. Malola, **H. Häkkinen**, B.K. Teo, Y. Cao and N. Zheng, ”Solvent-mediated assembly of atom-precise gold-silver nanoclusters to semiconducting one-dimensional materials”, *Nature Comm.* **11**, 2229 (2020).
- (238) K. Salorinne, R.W.Y. Man, P.A. Lummis, M. Sabooni Asre Hazer, S. Malola, J.C.H. Yim, A.J. Veinot, W. Zhou, **H. Häkkinen**, M. Nambo and C.M. Crudden, ”Synthesis and properties of an Au₆ cluster supported by a mixed N-heterocyclic carbene-thiolate ligand. “, *Chem Comm.* (2020).
- (239) H. Shen et al, ”Solubility-Driven Isolation of a Metastable Nonagold Cluster with Body-Centered Cubic Structure: Electronic Control of Cluster Stereochemistry”, *Chem – Eur J* (accepted) <https://doi.org/10.1002/chem.202001753>
- (240) A. Pihlajamäki, J. Hämäläinen, J. Linja, P. Nieminen, S. Malola, T. Kärkkäinen and **H. Häkkinen**, ”Monte Carlo Simulations of Au₃₈(SR)₂₄ Nanocluster Using Distance-Based Machine Learning Methods”, *J. Phys. Chem A* (2020). <https://pubs.acs.org/doi/pdf/10.1021/acs.jpca.0c01512>

(241) E. Selenius, S. Malola, M. Kuisma and **H. Häkkinen**, "Charge transfer plasmons in dimers of electron clusters", J. Phys. Chem. C (2020) <https://pubs.acs.org/doi/10.1021/acs.jpcc.0c02889>

B. Non-reviewed scientific articles (reviews and book chapters)

- (1) J. Merikoski, **H. Häkkinen**, M. Manninen, J. Timonen and K. Kaski, "Disordering mechanisms of the Cu(110) surface", Int. J. Mod. Phys. B **8**, 3175-3204 (1994).
- (2) **H. Häkkinen** and M. Manninen, "Metal cluster – surface interaction: Simple models and *ab initio* calculations", pp. 326-346 in "Theory of Atomic and Molecular Clusters with a Glimpse at Experiments", edited by J. Jellinek (Springer, Berlin 1999).
- (3) **H. Häkkinen**, "Ligand-protected gold clusters as superatoms – insights from theory and computations", chapter in "Nanoparticles", edited by R. Johnston and J. Wilcoxon, in series Frontiers of Nanoscience (Elsevier 2012).
- (4) **H. Häkkinen**, "When the size matters: theoretical studies of gold nanoclusters in various chemical environments", chapter in "Gold nanoparticles for physics, chemistry and biology", edited by Catherine Louis and Olivier Pluchery (World Scientific 2012, Second Edition 2017)
- (5) **H. Häkkinen**, "Superatom model for ligand-stabilized metal nanoclusters", chapter in "Protected Metal Clusters: From Fundamentals to Applications", edited by H. Häkkinen and T. Tsukuda, Elsevier (2015).
- (6) S. Malola and **H. Häkkinen**, "How many gold atoms make gold metal?", Feature Article in Europhysics News 46/4 (2015), DOI:10.1051/epn/2015402.
- (7) **H. Häkkinen**, A. Rosen, O. Echt and M. Pettersson, "ISSPIC XVIII: International symposium on small particles and inorganic clusters", J. Phys. Chem. C **121**, 10629-10631 (2017).
- (8) **H. Häkkinen**, "Au₁₀₂(pMBA)₄₄ nanocluster, a superatom suitable for bio-applications", Proc. SPIE **10174**, 1017402 (2016).

C. Scientific books

- (1) T. Tsukuda and **H. Häkkinen** (editors): "Protected Metal Clusters: From Fundamentals to Applications" (Elsevier, Amsterdam 2015).

G. Theses

- H. Häkkinen**, "Effective medium studies of defects in metals", PhD Thesis, University of Jyväskylä, 1991.

Submitted manuscripts:

M.F. Matus, S. Malola, E. Kinder Bonilla, B.M. Barngrover, C.M. Aikens and **H. Häkkinen**, "A topological isomer of the Au₂₅(SR)₁₈(-) nanocluster", submitted to Chem. Comm. (2020).