# CHEM0028: Concepts in Computational Chemistry

View Online

@article{Ackermann_Gale_Catlow_1997, title={Interaction of Methane with a [Li] Center on MgO(100):  HF, Post-HF, and DFT Cluster Model Studies}, volume={101}, url={https://contentstore.cla.co.uk/secure/link?id=e5196124-050c-f011-90cc-c5989c4ef87d}, DOI={10.1021/jp972198o}, number={48}, journal={The Journal of Physical Chemistry B}, author={Ackermann, L. and Gale, J. D. and Catlow, C. R. A.}, year={1997}, month={Nov}, pages={10028–10034} }

@article{Arndt_Laugel_Levchenko_Horn_Baerns_Scheffler_Schlögl_Schomäcker_2011, title={A Critical Assessment of Li/MgO-Based Catalysts for the Oxidative Coupling of Methane}, volume={53}, DOI={10.1080/01614940.2011.613330}, number={4}, journal={Catalysis Reviews}, author={Arndt, Sebastian and Laugel, Guillaume and Levchenko, Sergey and Horn, Raimund and Baerns, Manfred and Scheffler, Matthias and Schlögl, Robert and Schomäcker, Reinhard}, year={2011}, month={Oct}, pages={424–514} }

@book{Atkins_De Paula_2014, address={Oxford}, edition={Tenth edition}, title={Atkins' physical chemistry}, publisher={Oxford University Press}, author={Atkins, P. W. and De Paula, Julio}, year={2014} }

@book{Atkins_De Paula_Friedman_2009, address={Oxford}, title={Quanta, matter, and change: a molecular approach to physical chemistry}, publisher={Oxford University Press}, author={Atkins, P. W. and De Paula, Julio and Friedman, Ronald}, year={2009} }

@book{Bladon_Gorton_Hammond_2012, address={Cambridge}, title={Molecular modelling: computational chemistry demystified}, publisher={RSC Publishing}, author={Bladon, Peter and Gorton, John E. and Hammond, Robert B.}, year={2012} }

@article{C. R. A. Catlow, S. A. French, A. A. Sokol and J. M. Thomas_2005, title={Computational Approaches to the Determination of Active Site Structures and Reaction Mechanisms in Heterogeneous Catalysts}, volume={363}, url={http://www.jstor.org/stable/30039617?seq=19#page_scan_tab_contents}, number={1829}, journal={Philosophical Transactions: Mathematical, Physical and Engineering Sciences}, author={C. R. A. Catlow, S. A. French, A. A. Sokol and J. M. Thomas}, year={2005}, pages={913–936} }

@article{Deglmann_SchÃ¤fer_Lennartz_2015, title={Application of quantum calculations in the chemical industry-An overview}, volume={115}, DOI={10.1002/qua.24811}, number={3}, journal={International Journal of Quantum Chemistry}, author={Deglmann, Peter and SchÃ¤fer, Ansgar and Lennartz, Christian}, year={2015}, month={Feb},

pages={107–136} }

@book{Frenkel_Smit_1996, address={San Diego}, title={Understanding molecular simulation: from algorithms to applications}, publisher={Academic Press}, author={Frenkel, Daan and Smit, Berend}, year={1996} }

@book{Frenkel_Smit_2002, address={San Diego, Calif}, edition={2nd ed}, title={Understanding molecular simulation: from algorithms to applications}, volume={Computational science}, publisher={Academic Press}, author={Frenkel, Daan and Smit, Berend}, year={2002} }

@article{Frenkel_Smit_Ratner_1997, title={Understanding Molecular Simulation: From Algorithms to Applications}, volume={50}, DOI={10.1063/1.881812}, number={7}, journal={Physics Today}, author={Frenkel, Daan and Smit, Berend and Ratner, Mark A.}, year={1997} }

@article{Ganose_Scanlon_2016, title={Band gap and work function tailoring of SnO for improved transparent conducting ability in photovoltaics}, volume={4}, DOI={10.1039/C5TC04089B}, number={7}, journal={J. Mater. Chem. C}, author={Ganose, Alex M. and Scanlon, David O.}, year={2016}, pages={1467–1475} }

@book{Goodman_1998, address={Cambridge}, title={Chemical applications of molecular modelling}, publisher={Royal Society of Chemistry}, author={Goodman, Jonathan M.}, year={1998} }

@book{Jensen_2007, address={Chichester}, edition={2nd ed}, title={Introduction to computational chemistry}, publisher={John Wiley & Sons}, author={Jensen, Frank}, year={2007} }

@article{Lau_Hunt_Müller_Jackson_Ford_2015, title={Water droplet excess free energy determined by cluster mitosis using guided molecular dynamics}, volume={143}, DOI={10.1063/1.4935198}, number={24}, journal={The Journal of Chemical Physics}, author={Lau, Gabriel V. and Hunt, Patricia A. and Müller, Erich A. and Jackson, George and Ford, Ian J.}, year={2015}, month={Dec} }

@book{Leach_2001, address={Harlow, England}, edition={Second edition}, title={Molecular modelling: principles and applications}, publisher={Pearson}, author={Leach, Andrew R.}, year={2001} }

@article{Price_Reutzel-Edens_2016, title={The potential of computed crystal energy landscapes to aid solid-form development}, volume={21}, DOI={10.1016/j.drudis.2016.01.014}, number={6}, journal={Drug Discovery Today}, author={Price, Sarah L. and Reutzel-Edens, Susan M.}, year={2016}, month={Jun}, pages={912–923} }

@article{Scanlon_Walsh_Morgan_Nolan_Fearon_Watson_2007, title={Surface Sensitivity in Lithium-Doping of MgO: A Density Functional Theory Study with Correction for on-Site Coulomb Interactions}, volume={111}, DOI={10.1021/jp070200y}, number={22}, journal={Journal of Physical Chemistry C}, author={Scanlon, D.O. and Walsh, A. and Morgan, B.J. and Nolan, M. and Fearon, J. and Watson, G.W.}, year={2007}, month={Jun}, pages={7971–7979} }

@inbook{Silbey_Alberty_Bawendi_Alberty_2005, address={Hoboken, N.J.}, edition={4th ed}, title={Alberti & Silbey Chapter on Quantum Chemistry}, booktitle={Physical chemistry}, publisher={Wiley}, author={Silbey, Robert J. and Alberty, Robert A. and Bawendi, Moungi Gabriel and Alberty, Robert A.}, year={2005} }

@article{Stiakaki_Tsipis_Tsipis_Xanthopoulos_1996, title={Theoretical aspects of methane chemisorption on MgO surfaces. Modelling of impurity-induced trapping of a hole, surface defects and site dependence of methane chemisorption on (MgO)9,12 clusters}, volume={92}, DOI={10.1039/ft9969202765}, number={15}, journal={Journal of the Chemical Society, Faraday Transactions}, author={Stiakaki, Maria-Aglaia D. and Tsipis, Athanasios C. and Tsipis, Constantions A. and Xanthopoulos, Constantinos E.}, year={1996} }

@article{Tribello_Slater_Salzmann_2006, title={A Blind Structure Prediction of Ice XIV}, volume={128}, url={https://contentstore.cla.co.uk/secure/link?id=24d6c08f-040c-f011-90cc-c5989c4ef87d}, DOI={10.1021/ja0630902}, number={39}, journal={Journal of the American Chemical Society}, author={Tribello, Gareth A. and Slater, Ben and Salzmann, Christoph G.}, year={2006}, month={Oct}, pages={12594–12595} }

@misc{Theory and Applications in Computational Chemistry, url={http://www.tacc2012.org/Proceedings.html} }

@misc{The Nobel Prize in Chemistry 1998 - Summary, url={http://www.nobelprize.org/nobel_prizes/chemistry/laureates/1998/advanced.html} }

@misc{John Pople Nobel Lecture - HF methods, url={https://www.nobelprize.org/uploads/2018/06/pople-lecture.pdf} }

@misc{Walter Kohn Nobel Lecture - DFT, url={https://www.nobelprize.org/uploads/2018/06/kohn-lecture.pdf} }