

CHEM0028: Concepts in Computational Chemistry

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1.

Goodman JM. Chemical applications of molecular modelling. Cambridge: Royal Society of Chemistry; 1998.

2.

Jensen F. Introduction to computational chemistry. 2nd ed. Chichester: John Wiley & Sons; 2007.

3.

Frenkel D, Smit B. Understanding molecular simulation: from algorithms to applications. 2nd ed. San Diego, Calif: Academic Press; 2002.

4.

Frenkel D, Smit B. Understanding molecular simulation: from algorithms to applications. San Diego: Academic Press; 1996.

5.

Frenkel D, Smit B, Ratner MA. Understanding Molecular Simulation: From Algorithms to Applications. Physics Today. 1997;50(7).

6.

Bladon P, Gorton JE, Hammond RB. Molecular modelling: computational chemistry

demystified. Cambridge: RSC Publishing; 2012.

7.

Theory and Applications in Computational Chemistry [Internet]. Available from: <http://www.tacc2012.org/Proceedings.html>

8.

Lau GV, Hunt PA, Müller EA, Jackson G, Ford IJ. Water droplet excess free energy determined by cluster mitosis using guided molecular dynamics. *The Journal of Chemical Physics*. 2015 Dec 28;143(24).

9.

Tribello GA, Slater B, Salzmann CG. A Blind Structure Prediction of Ice XIV. *Journal of the American Chemical Society* [Internet]. 2006 Oct;128(39):12594–12595. Available from: <https://contentstore.cla.co.uk/secure/link?id=24d6c08f-040c-f011-90cc-c5989c4ef87d>

10.

Price SL, Reutzel-Edens SM. The potential of computed crystal energy landscapes to aid solid-form development. *Drug Discovery Today*. 2016 Jun;21(6):912–923.

11.

Silbey RJ, Alberty RA, Bawendi MG, Alberty RA. Alberty & Silbey Chapter on Quantum Chemistry. *Physical chemistry*. 4th ed. Hoboken, N.J.: Wiley; 2005.

12.

Atkins PW, De Paula J. *Atkins' physical chemistry*. Tenth edition. Oxford: Oxford University Press; 2014.

13.

Deglmann P, SchÄrfer A, Lennartz C. Application of quantum calculations in the chemical

industry-An overview. International Journal of Quantum Chemistry. 2015 Feb 5;115(3):107–136.

14.

Leach AR. Molecular modelling: principles and applications. Second edition. Harlow, England: Pearson; 2001.

15.

Atkins PW, De Paula J, Friedman R. Quanta, matter, and change: a molecular approach to physical chemistry. Oxford: Oxford University Press; 2009.

16.

Arndt S, Laugel G, Levchenko S, Horn R, Baerns M, Scheffler M, Schlögl R, Schomäcker R. A Critical Assessment of Li/MgO-Based Catalysts for the Oxidative Coupling of Methane. Catalysis Reviews. 2011 Oct;53(4):424–514.

17.

Ackermann L, Gale JD, Catlow CRA. Interaction of Methane with a [Li] Center on MgO(100): HF, Post-HF, and DFT Cluster Model Studies. The Journal of Physical Chemistry B [Internet]. 1997 Nov;101(48):10028–10034. Available from: <https://contentstore.cla.co.uk/secure/link?id=e5196124-050c-f011-90cc-c5989c4ef87d>

18.

C. R. A. Catlow, S. A. French, A. A. Sokol and J. M. Thomas. Computational Approaches to the Determination of Active Site Structures and Reaction Mechanisms in Heterogeneous Catalysts. Philosophical Transactions: Mathematical, Physical and Engineering Sciences [Internet]. 2005;363(1829):913–936. Available from: http://www.jstor.org/stable/30039617?seq=19#page_scan_tab_contents

19.

Stiakaki MAD, Tsipis AC, Tsipis CA, Xanthopoulos CE. 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. Journal of

the Chemical Society, Faraday Transactions. 1996;92(15).

20.

Scanlon DO, Walsh A, Morgan BJ, Nolan M, Fearon J, Watson GW. Surface Sensitivity in Lithium-Doping of MgO: A Density Functional Theory Study with Correction for on-Site Coulomb Interactions. Journal of Physical Chemistry C. 2007 Jun 7;111(22):7971–7979.

21.

The Nobel Prize in Chemistry 1998 - Summary [Internet]. Available from:
http://www.nobelprize.org/nobel_prizes/chemistry/laureates/1998/advanced.html

22.

John Pople Nobel Lecture - HF methods [Internet]. Available from:
<https://www.nobelprize.org/uploads/2018/06/pople-lecture.pdf>

23.

Walter Kohn Nobel Lecture - DFT [Internet]. Available from:
<https://www.nobelprize.org/uploads/2018/06/kohn-lecture.pdf>

24.

Ganose AM, Scanlon DO. Band gap and work function tailoring of SnO₂ for improved transparent conducting ability in photovoltaics. J Mater Chem C. 2016;4(7):1467–1475.

for