

CHEM0028: Concepts in Computational Chemistry

[View Online](#)

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. doi:10.1063/1.881812

6

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

demystified. Cambridge: : RSC Publishing 2012.

7

Theory and Applications in Computational Chemistry.
<http://www.tacc2012.org/Proceedings.html>

8

Lau GV, Hunt PA, Müller EA, et al. Water droplet excess free energy determined by cluster mitosis using guided molecular dynamics. *The Journal of Chemical Physics* 2015; **143**. doi:10.1063/1.4935198

9

Tribello GA, Slater B, Salzmann CG. A Blind Structure Prediction of Ice XIV. *Journal of the American Chemical Society* 2006; **128**:12594–5. doi:10.1021/ja0630902

10

Price SL, Reutzel-Edens SM. The potential of computed crystal energy landscapes to aid solid-form development. *Drug Discovery Today* 2016; **21**:912–23.
doi:10.1016/j.drudis.2016.01.014

11

Silbey RJ, Albert RA, Bawendi MG, et al. Alberti & Silbey Chapter on Quantum Chemistry. In: Physical chemistry. Hoboken, N.J.: : Wiley 2005.

12

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

13

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

industry-An overview. International Journal of Quantum Chemistry 2015; **115**:107–36.
doi:10.1002/qua.24811

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, et al. A Critical Assessment of Li/MgO-Based Catalysts for the Oxidative Coupling of Methane. Catalysis Reviews 2011; **53**:424–514.
doi:10.1080/01614940.2011.613330

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 1997; **101**:10028–34. doi:10.1021/jp9721980

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 2005; **363**:913–36. http://www.jstor.org/stable/30039617?seq=19#page_scan_contents

19

Stiakaki M-AD, Tsipis AC, Tsipis CA, et al. 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**. doi:10.1039/ft9969202765

20

Scanlon DO, Walsh A, Morgan BJ, et al. 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; **111**:7971–9. doi:10.1021/jp070200y

21

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

22

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

23

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

24

Ganose AM, Scanlon DO. Band gap and work function tailoring of SnO for improved transparent conducting ability in photovoltaics. *J Mater Chem C* 2016; **4**:1467–75. doi:10.1039/C5TC04089B