

CHEM0028: Concepts in Computational Chemistry

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1.

Goodman, J. M. Chemical applications of molecular modelling. (Royal Society of Chemistry, 1998).

2.

Jensen, F. Introduction to computational chemistry. (John Wiley & Sons, 2007).

3.

Frenkel, D. & Smit, B. Understanding molecular simulation: from algorithms to applications. vol. Computational science (Academic Press, 2002).

4.

Frenkel, D. & Smit, B. Understanding molecular simulation: from algorithms to applications. (Academic Press, 1996).

5.

Frenkel, D., Smit, B. & Ratner, M. A. Understanding Molecular Simulation: From Algorithms to Applications. *Physics Today* **50**, (1997).

6.

Bladon, P., Gorton, J. E. & Hammond, R. B. Molecular modelling: computational chemistry demystified. (RSC Publishing, 2012).

7.

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

8.

Lau, G. V., Hunt, P. A., Müller, E. A., Jackson, G. & Ford, I. J. Water droplet excess free energy determined by cluster mitosis using guided molecular dynamics. *The Journal of Chemical Physics* **143**, (2015).

9.

Tribello, G. A., Slater, B. & Salzmann, C. G. A Blind Structure Prediction of Ice XIV. *Journal of the American Chemical Society* **128**, 12594–12595 (2006).

10.

Price, S. L. & Reutzel-Edens, S. M. The potential of computed crystal energy landscapes to aid solid-form development. *Drug Discovery Today* **21**, 912–923 (2016).

11.

Silbey, R. J., Alberty, R. A., Bawendi, M. G. & Alberty, R. A. Alberty & Silbey Chapter on Quantum Chemistry. in *Physical chemistry* (Wiley, 2005).

12.

Atkins, P. W. & De Paula, J. *Atkins' physical chemistry*. (Oxford University Press, 2014).

13.

Deglmann, P., Schäfer, A. & Lennartz, C. Application of quantum calculations in the chemical industry-An overview. *International Journal of Quantum Chemistry* **115**, 107–136 (2015).

14.

Leach, A. R. Molecular modelling: principles and applications. (Pearson, 2001).

15.

Atkins, P. W., De Paula, J. & Friedman, R. Quanta, matter, and change: a molecular approach to physical chemistry. (Oxford University Press, 2009).

16.

Arndt, S. et al. A Critical Assessment of Li/MgO-Based Catalysts for the Oxidative Coupling of Methane. *Catalysis Reviews* **53**, 424–514 (2011).

17.

Ackermann, L., Gale, J. D. & Catlow, C. R. A. Interaction of Methane with a [Li] Center on MgO(100): HF, Post-HF, and DFT Cluster Model Studies. *The Journal of Physical Chemistry B* **101**, 10028–10034 (1997).

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* **363**, 913–936 (2005).

19.

Stiakaki, M.-A. D., Tsipis, A. C., Tsipis, C. A. & Xanthopoulos, C. E. 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* **92**, (1996).

20.

Scanlon, D. O. 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* **111**, 7971–7979 (2007).

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.

23.

Walter Kohn Nobel Lecture - DFT.

24.

Ganose, A. M. & Scanlon, D. O. Band gap and work function tailoring of SnO₂ for improved transparent conducting ability in photovoltaics. *J. Mater. Chem. C* **4**, 1467–1475 (2016).