

CHEM0028: Concepts in Computational Chemistry

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1.

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

2.

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

3.

Frenkel, D., Smit, B.: Understanding molecular simulation: from algorithms to applications. Academic Press, San Diego, Calif (2002).

4.

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

5.

Frenkel, D., Smit, B., Ratner, M.A.: Understanding Molecular Simulation: From Algorithms to Applications. Physics Today. 50, (1997). <https://doi.org/10.1063/1.881812>.

6.

Bladon, P., Gorton, J.E., Hammond, R.B.: Molecular modelling: computational chemistry

demystified. RSC Publishing, Cambridge (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). <https://doi.org/10.1063/1.4935198>.

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).
<https://doi.org/10.1021/ja0630902>.

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).
<https://doi.org/10.1016/j.drudis.2016.01.014>.

11.

Silbey, R.J., Alberty, R.A., Bawendi, M.G., Alberty, R.A.: Alberti & Silbey Chapter on Quantum Chemistry. In: *Physical chemistry*. Wiley, Hoboken, N.J. (2005).

12.

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

13.

Deglmann, P., SchÄxfer, A., Lennartz, C.: Application of quantum calculations in the chemical industry-An overview. *International Journal of Quantum Chemistry*. 115, 107–136 (2015). <https://doi.org/10.1002/qua.24811>.

14.

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

15.

Atkins, P.W., De Paula, J., Friedman, R.: *Quanta, matter, and change: a molecular approach to physical chemistry*. Oxford University Press, Oxford (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*. 53, 424–514 (2011). <https://doi.org/10.1080/01614940.2011.613330>.

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). <https://doi.org/10.1021/jp972198o>.

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).
<https://doi.org/10.1039/ft9969202765>.

20.

Scanlon, D.O., Walsh, A., Morgan, B.J., Nolan, M., Fearon, J., Watson, G.W.: 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).
<https://doi.org/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, A.M., Scanlon, D.O.: Band gap and work function tailoring of SnO for improved transparent conducting ability in photovoltaics. *J. Mater. Chem. C*. 4, 1467–1475 (2016). <https://doi.org/10.1039/C5TC04089B>.