

Reading list for Theoretical and computational tools for chemists, TNSM02, 2026

Books

Atkins, P. W., De Paula, Julio, Keeler, James, (2023) *Atkins' physical chemistry*. Twelfth edition Oxford : Oxford University Press, [2023]
ISBN: 9780198847816

Frenkel, Daan, Smit, Berend, (2023) *Understanding molecular simulation : from algorithms to applications*. Third edition. London, United Kingdom ; San Diego, CA, United States ; Cambridge, MA, United States ; Kidlington, Oxford, United Kingdom : Elsevier, Academic Press, an Imprint of Elsevier, [2023]
ISBN: 0323913180, 9780323913188

Sholl, David S., Steckel, Janice A., (2009) *Density functional theory. a practical introduction*. [Elektronisk resurs] Hoboken, N.J. : Wiley, c2009.

Ullrich, Carsten A., (2012) *Time-dependent density-functional theory : concepts and applications*
ISBN: 9780199563029, 9780198841937, 0199563020, 0198841930