



ROMANIAN ACADEMY
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Topics and Bibliography for the Competition

Topics:

- o Fundamentals of quantum chemistry and computational chemistry.
- o Electronic structure calculation methods (Hartree–Fock, DFT – general concepts).
- o Molecular dynamics – principles and applications.
- o Use of molecular modeling software and interpretation of results.
 - Applications of computational chemistry in the study of biomolecules, materials, and chemical processes.

Selected bibliography:

- o [BioMat4CAST Project Website](#), including scientific publications and educational materials available on the project website.

Optional:

1. **Leach, A. R.** *Molecular Modelling: Principles and Applications*, 2nd Edition. Pearson Education, 2001.
2. **Jensen, F.** *Introduction to Computational Chemistry*, 3rd Edition. John Wiley & Sons, 2017.
3. **Cramer, C. J.** *Essentials of Computational Chemistry: Theories and Models*, 2nd Edition. John Wiley & Sons, 2004.