

Lecture 0: The Context of Computational Chemistry

Find an article in the current literature that uses quantum chemical calculations in some way to address some chemical or materials problem.

Good potential sources include *J. Am. Chem. Soc.*, *J. Phys. Chem.*, *Science*, *Angew. Chemie*, *Phys. Chem. Chem. Phys.*, *Inorg. Chem.*, *Phys. Rev.*, *Nature*, *J. Catal.*,

1. Give the full citation of your article, including authors, title, journal, year, volume, pages, and doi (digital object identifier).
2. In just two to three sentences, what question do the authors try to answer using their calculations?
3. In just two to three sentences, what answer do they arrive at?