Simulation of materials from first-principles: successes, challenges and application to vibrational spectroscopies

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I will provide an introduction to the fundamentals of electronic-structure methods, their current capabilities and limitations, highlighting which materials properties can be calculated, and with which accuracy. A special care will be dedicated to vibrational spectroscopies.

Suggested reading: N. Marzari, A. Ferretti, and C. Wolverton, Nature Materials 20, 736 (2021).