

ID: P1.22

Title: QMC calculations on ThO molecule and ThO₂ crystal

Name: Hu, Shuming

Affiliation: NCSU

Quantum Monte Carlo calculations on ThO molecule and ThO₂ crystal with Stuttgart RLC/RSC ECP. Different sizes of simulation cell has been used for crystal calculations. Fixed-Node diffusion Monte Carlo has been used to calculate ground state and excited states energy as well as other properties. We compare our results with experimental data, and we assess the accuracy of trial wavefunctions with regard to fixed-node approximation.