Goldschmidt 2026 Abstract
https://doi.org/10.46427/gold2026.35301

# Quantum Chemistry at Extreme Pressures

ERIKA MAGNUSSON[1], MICHELANGELO BOVOLONI[1,2], BO CHEN[3] AND **MARTIN RAHM**[1]

[1]Chalmers University of Technology
[2]Politecnico di Milano
[3]Donostia International Physics Center

Quantum-mechanical modeling of chemistry at gigapascal pressures can greatly aid our understanding of planetary interiors, yet most such work targets extended crystalline phases treated with periodic boundary conditions and density functional approximations. This presentation outlines the basics of an established alternative approach, the Extreme-Pressure Polarizable Continuum Model (XP-PCM), which describes the confining environment as an isotropic non-reactive medium. XP-PCM thereby enables systematic, high-accuracy studies of pressure-induced changes in atomic and molecular characteristics, including electronegativity, size, and electronic configurations. Emphasis will be placed on qualitative predictions of evolving bonding patterns under compression relevant for deep planetary environments, along with a brief overview of recent technical developments.