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First−principle molecular−dynamic simulation of minerals at deep Earth's temperatures and pressures

Sandro Scandolo[*]

Department of Chemistry and Department of Geosciences, Princeton University (USA)

Lack of direct access and difficulties in reproducing in the laboratory the extreme temperature and pressure conditions that characterise the Earth's deep interior make first−principle molecular dynamics simulations an ideal tool to study the properties of deep−Earth minerals. In this talk I will present our findings on the properties of solid and liquid iron at Earth's core pressures and temperatures, and more recent results on the properties of MgO and $MgSiO_3$, the major components of the Earth's lower mantle. In particular, I will address the question of whether $MgSiO_3$, an antiferrodistorted perovskite structure at low temperatures, undergoes temperature−induced structural transitions to higher−symmetry phases at Earth's mantle temperatures.

Work done in collaboration with S. Bernard, G. Chiarotti, A. Laio, P. Tangney, and E. Tosatti.

(*) on sabbatical leave from the International School for Advanced Studies (SISSA), Trieste (Italy)