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The determination of thermal and structural state of the lower mantle and core via ab initio molecular dynamics (Louis Néel Medal Lecture)

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Atomic-scale materials modelling based on first-principles quantum mechanics (ab initio methods) is playing an important role in the science of the Earth and the other planets. The basic theory of this kind of modelling will be outlined, and it will be shown how it can be a applied in a variety of different ways to probe the thermodynamics, structure and transport properties of both solids and liquids under extreme conditions. Specifically, recent work on constraining the structural and thermal properties of the lowermost mantle (D") will be discussed. A number of theories have been proposed to explain the origin of the variety of characteristics of this seismically observed layer, including core–mantle interaction, the presence of remnants of subducted material, and that D" is the site of a mineral phase transformation. This final possibility has been rejuvenated by recent evidence for a phase change in $MgSiO_3$ perovskite (thought to be the most prevalent phase in the lower mantle) at near core–mantle boundary temperature and pressure conditions. We have explored the efficacy of this 'post-perovskite' phase to explain the seismic properties of the lowermost mantle through coupled ab initio molecular dynamics and seismic modelling of perovskite and post-perovskite polymorphs of $MgSiO_3$, performed at lowermost mantle temperatures and pressures. We have found that a post-perovskite model can explain the topography and location of the D" discontinuity, apparent differences in compressional- and shear wave models and the observation of a deeper, weaker discontinuity. Our calculations show that the regional variations in lower-mantle shear-wave anisotropy are consistent with the proposed phase change in $MgSiO_3$ perovskite.