Novel High-pressure Phases: Theory and Experiment

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Searching for new materials and new crystal structures at high pressures and temperatures is important for fundamental physics, for material sciences, and for understanding the structure and properties of planetary interiors. State-of-the-art computer simulations can fruitfully complement or even guide experimental efforts in this direction. Here, we present recent joint theoretical/experimental discoveries of new geophysically important phases of MgSiO₃ [1-3] and Al₂O₃[4] with implications for the structure, dynamics, electrical conductivity, rheology and seismic signatures of the Earth's lowermost mantle.

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