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Formation and superconductivity of hydrides under pressure¹

DUCK YOUNG KIM, TCM group, Cavendish laboratory, University of Cambridge, UK, RALPH H. SCHEICHER, Uppsala University, Sweden, CHRIS J. PICKARD, University College London, UK, RICHARD J. NEEDS, TCM group, Cavendish laboratory, University of Cambridge, UK, RAJEEV AHUJA, Uppsala University, Sweden — Hydrogen is the lightest and smallest element in the periodic table. Despite its simplest electronic structure, enormous complexity can arise when hydrogen participates in the formation of solids. Pressure as a controllable parameter can provide an excellent platform to investigate novel physics of hydrides because it can induce structural transformation and even changes in stoichiometry accompanied with phenomena such as metallization and superconductivity. In this presentation, we will briefly overview contemporary high-pressure research on hydrides and show our most recent results on predicting crystal structures of metal hydrides under pressure using ab initio random structure searching. Our findings allow for a better understanding of pressure-induced metallization/superconductivity in hydrides which can help to shed light on recent observations of pressure-induced metallization and superconductivity in hydrogen-rich materials.

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