Hydrogen rich materials for hydrogen storage under high pressure

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The purpose of this talk is to provide an overview of the most recent theoretical studies undertaken by us in the field of hydrogen storage materials research with the focus “how high pressure” can play an important role in search and design of new hydrogen storage materials. On specific examples, the application of density functional theory calculations and molecular dynamics simulations will be illustrated to show how these computational methods can be of great use in the effort to reach a better understanding of materials and to guide the search for new promising candidates. Systems to be discussed include: tri-hydrides, light-metal hydrides, with “classics” such as NaAlH4 and MgH2, and high-surface porous materials.