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**High pressure hydrogen stabilised by quantum nuclear motion**[1]
RICHARD NEEDS, BARTOMEU MONSERRAT, CHRIS PICKARD, University of Cambridge — Hydrogen under extreme pressures is of fundamental interest, as it might exhibit exotic physical phenomena, and of practical interest, as it is a major component of many astrophysical objects. Structure searches have been successful at identifying promising candidates for the known phases of high pressure hydrogen. However, these searches have so far been restricted to the location of minima of the potential energy landscape. In this talk, we will describe a new structure searching method, "saddle-point ab initio random structure searching" (sp-AIRSS), that allows us to identify structures associated with saddle points of the potential energy landscape. Using sp-AIRSS, we find two new high-pressure hydrogen structures that exhibit a harmonic dynamical instability, but quantum and thermal anharmonic motion render them dynamically stable. These structures are formed by mixed layers of strongly and softly bound hydrogen molecules, and become thermodynamically competitive at the highest pressures reached in experiment. The experimental implications of these new structures will also be discussed.

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