

SMP045-01

Room:301B

Time:May 24 14:15-14:30

Pressure-induced intermolecular interactions in crystalline silane-hydrogen

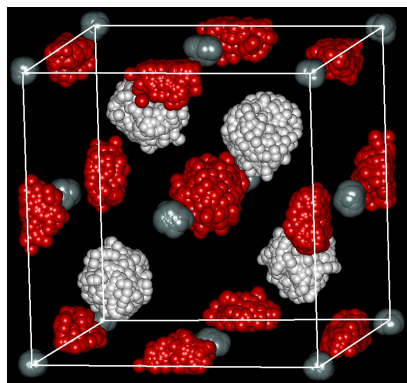
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The structure and dynamics of a recently discovered solid silane-hydrogen complex under high pressure are elucidated with first-principles molecular dynamics calculations. A structure with orientationally disordered silane and hydrogen with their centers of mass arranged in a distinctive manner are found. Natural bond orbital analysis reveals that perturbative donor-acceptor interactions between the two molecular species are enhanced by pressure. The experimentally observed anticorrelated pressure-frequency dependency is a consequence of these novel interactions. Possibility of finding such solid silane-hydrogen complex inside of Jupiter is discussed.

<http://www.iitaka.org/~neutron/theory.html>

<http://www.rikenresearch.riken.jp/eng/research/6495>



Keywords: hydrogen, silane, high pressure, intermolecular interaction, vibron, molecular dynamics