

Novel modulated structure of superconducting hydrogen sulfide

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First Principles metadynamics and molecular dynamics calculations revealed a metastable modulated structure with high proton mobility and a diffraction pattern matches the experimental measurements at 200 GPa and 200K. The structure, obtained from compression of the low pressure Pmc21 phase, is consisted of a sublattice of rectangular meander SH- chains with molecular-like H3S+ and stacked alternately in tetragonal and cubic slabs forming a long-period modulated crystal. The novel structure offers a new perspective on the possible origin of the very high superconductivity in which the conducting electrons in the SH chains are perturbed by the fluxional motions of the H3S resulting in strong electron-phonon couplings.

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