

Abstract Submitted
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An effective 2-band e_g model of sulfur hydride H_3S for high- T_C superconductivity KAZUTAKA NISHIGUCHI, SHINGO TERANISHI, SATOAKI MIYAO, GOH MATSUSHITA, KOICHI KUSAKABE, Graduate School of Engineering Science, Osaka University — To understand high transition temperature (T_C) superconductivity in sulfur hydride H_3S , we propose an effective 2-band model having the e_g symmetry as the minimal model for H_3S . Two e_g orbitals centered on a sulfur S atom are chosen for the smallest representation of relevant bands with the van-Hove singularity around the Fermi levels except for the Γ -centered small hole pockets by the sulfur $3p$ orbitals. By using the maximally localized Wannier functions, we derive the minimal effective model preserving the body-centered cubic (bcc) crystal symmetry of the H_3S phase having the highest T_C (~ 203 K under pressures) among the other polymorphs of H_3S .

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