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van Hove Singularities and Spectral Smearing in High Temperature Superconducting H_3S[1] YUNDI QUAN, Physics Department, UC Davis CAQS, Beijing Normal Univ., WARREN E. PICKETT, Physics Department, UC Davis — The superconducting phase of hydrogen sulfide at T_c=200 K observed by Drozdov and collaborators at pressures around 200 GPa is simple bcc $Im\bar{3}m$ H_3S reopens questions about what is achievable in high T_c. The various "extremes" that are involved – pressure, implying extreme reduction of volume, extremely high H phonon energy scale around 1400K, extremely high temperature for a superconductor – necessitate a close look at new issues raised by these characteristics in relation to high T_c. We have applied first principles methods to analyze the H_3S electronic structure, particularly the van Hove singularities (vHs) and the effect of sulfur. Focusing on the two closely spaced vHs near the Fermi level that give rise to the impressively sharp peak in the density of states, the implications of strong coupling Migdal-Eliashberg theory are assessed. The electron spectral density smearing due to virtual phonon emission and absorption, as done in earlier days for A15 superconductors, must be included explicitly to obtain accurate theoretical predictions and a correct understanding. Means for increasing T_c in H_3S-like materials will be mentioned.

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