

Quantum Monte Carlo method in high  $T_c$  sulfur hydrideR. Taureau<sup>a\*</sup>, M. Casula<sup>a\*\*</sup>

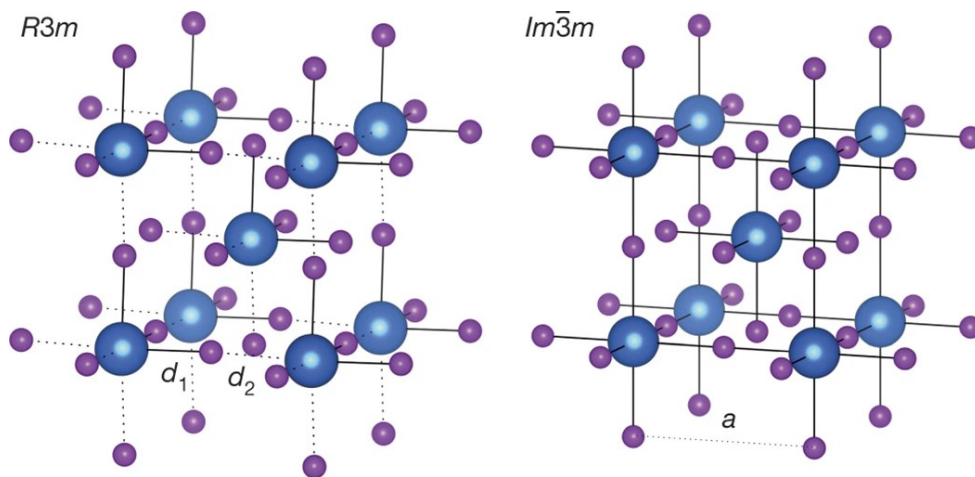
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$H_3S$  is one of the firstsly discovered hydride superconductors with very high  $T_c$  (203 K) [1]. This high  $T_c$  occurs around the  $R3m \rightarrow Im\bar{3}m$  phase transition peak at very high pressure (150 GPa). Current DFT methods fail to reproduce the location of the transition pressure and the experimental data [2]. In this work we investigate this transition with more advanced methods such as *Quantum Monte Carlo*, in order to get a more accurate description of the electronic correlations and reproduce these data.

[1] Drozdov, A., Eremets, M., Troyan, I. *et al. Nature* **525**, 73–76 (2015).

[2] Errea, I., Calandra, M., Pickard, C. *et al. Nature* **532**, 81–84 (2016).



**Figure 1** : H<sub>3</sub>S crystal representation, the high  $T_c$  is maximal when the transition occurs between these two close phases. In blue the hydrogen atoms, in purple the sulfur ones. (Source [2])