Quantum Monte Carlo method in high $T_c$ sulfur hydride

R. Taureau$^a$*, M. Casula$^{a**}$

*a. Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, CNRS UMR 7590,IRD UMR 206, MNHN, 4 Place Jussieu, 75252 Paris, France

* email: roomain.taureau@sorbonne-universite.fr, ** michele.casula@sorbonne-universite.fr

$H_3S$ 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-3m 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.


Figure 1: $H_3S$ 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])