

Superconductivity in molecular solids at high pressure

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Recently it was proposed that hydrogen rich metal alloys may be high temperature superconductors [1]. It was pointed out that the high pressure metallic phases of Group IVa hydrides are potential candidates. Following this suggestion, the optical properties of SiH_4 have been examined up to 218 GPa by experiment [2]. The results strongly suggest an insulator-metal transition at 80 GPa. Motivated by the experimental finding, theoretical electronic structure calculations were performed to explore possible high pressure phases of Group IVa SiH_4 and SnH_4 hydrides. Starting from ambient structures, First-Principle molecular dynamics simulations were used to identify stable high pressure polymorphs. The crystal structure, electronic and vibrational properties and the possibility of superconductivity behaviour in these novel high pressure structures will be presented and discussed.

References

[1] - N. W. Ashcroft Phys. Rev. Lett. **92**, 187002 (2004)

[2] - A.L. Ruoff, L. Sun, C. Zha and G. Stupian, AIRAPT, Proceedings, Karlsruhe (2005)