Carbon at extreme conditions

Sandro Scandolo [a]

[a] *The "Abdus Salam" International Centre for Theoretical Physics, Trieste, Italy.*

email:

The pressure-induced transformation of graphite into diamond, first reproduced in the laboratory in 1955, is now an industrial process with a global market worth $20 billions. In the graphite-diamond transformation pressure is used as an external force to induce the sp^2-sp^3 hybridization change. Extreme conditions of pressure and temperature such as those found in the interiors of planets can nowadays be reproduced routinely in the lab and can be used to explore novel chemical changes in carbon. Understanding such changes has far ranging implications in materials science, chemistry, planetary sciences, and geophysics. In this context, atomistic simulations based on density-functional theory play an important role [1]. I will present some recent updates on the phase diagram of carbon at TPa pressure [2] and discuss the mechanical stability of diamond under hydrostatic and strongly uniaxial compression [3]. I will also illustrate how extreme conditions affect the chemistry of carbon-bearing compounds such as CO_2 and CH_4. Specifically, I will describe the pressure-induced collapse of molecular CO_2 into extended covalently-bonded polymorphs [4] and the solvation, ionization, and full dissociation of methane in water under planetary conditions [5, 6].

[1]. A.R. Oganov, G.D. Price, S. Scandolo, Ab initio theory of planetary materials, Z. Kristallogr. 220 (2005) 531-548.

[2]. B.H. Cogollo-Olivo, J.A. Montoya, S. Scandolo, in preparation.

[3]. A.M.I. Bakhit, S. Mutisya, S. Scandolo, Raman frequencies of diamond under non-hydrostatic pressure, submitted.

[4]. B.H. Cogollo-Olivo, S. Biswas, S. Scandolo, J.A. Montoya, Ab initio Determination of the Phase Diagram of CO_2 at High Pressures and Temperatures, Phys. Rev. Lett. 124 (2020) 095701.

[5]. C.G. Pruteanu, V. Naden Robinson, N. Ansari, A. Hassanali, S. Scandolo, J.S. Loveday, Squeezing Oil into Water under Pressure: Inverting the Hydrophobic Effect, J. Phys. Chem. Lett. 11 (2020) 4826-4833.

[6]. M.S. Lee, S. Scandolo, Mixtures of planetary ices at extreme conditions, Nature Comm. 2 (2011) 1-5.