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Intercalated carbon materials at extreme conditions

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The high pressure and high temperature phase diagrams of intercalated carbon materials offer novel approaches for the engineering of new carbon functional materials. In this talk I will explore the structural, electronic, and vibrational properties of intercalated 2D fullerites and graphites when submitted to severe high pressure conditions. In graphite and fullerites, the graphene layers or the fullerenes molecules are held together in the crystal structure by the weak van der Waals forces and intercalation is easy due to the low energies involved. The guest-host charge transfer which may occur, results in profound modifications of the physico-chemical properties of the host. Applying external pressure to these materials provokes the contraction of bond lengths, leading to drastic changes such as sp2-sp3 C transitions, anisotropic and isotropic deformation, and insulator-metallic transformations. When the energetic landscape is favorable, the metastabilization of new forms of carbon allotropes at ambient conditions can occur.

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No

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