Theory of the carbon vacancy in silicon carbide

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Due to its outstanding properties, silicon carbide (SiC) is becoming the material of choice for high-voltage and high-power electronics. However, the presence of carbon vacancies in as-grown material has been the cause of device failures like low field effect mobility. Understanding the properties of this defect is a major challenge along the way to produce better material. Recently, our group performed state-of-the-art first-principles calculations using several hundreds of atoms and described with great accuracy the properties of electrons coupled to the nuclei around the defect. We were able to solve several unanswered issues raised by electron paramagnetic resonance, all of which were found to originate from a pseudo-Jahn-Teller effect driven by an internal crystal field. These results had excellent acceptance by the community. They actually stimulated other groups to design new experiments in order to verify some of our predictions.

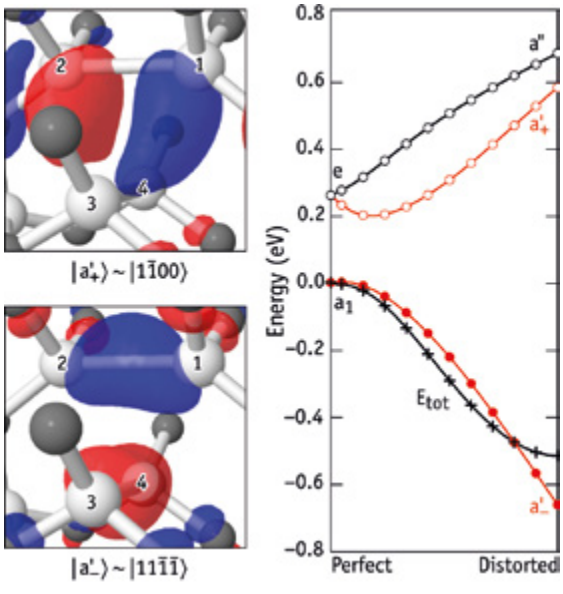

FIGURE 1
(Left) Shape of the highest occupied and lowest unoccupied Kohn-Sham orbitals of a neutral carbon vacancy in 4H-SiC. (Right) Evolution of the single-electron states in the gap as the structure changes from a perfect vacancy to the distorted ground state. Occupied and empty states are represented as solid and open circles, respectively. The total energy (E_{tot}) is shown as crosses. Figure adapted from Reference 2.

A wide and indirect band gap, high chemical and thermal stability, as well as radiation and electrical hardness, are among the merits that make silicon carbide (SiC) an outstanding material for high-voltage and high-power electronics [1]. Among several stable polytypes, the hex-agonal 4H-SiC has become the material of choice of the industry. However, the presence of carbon-related point defects in SiC, particularly carbon vacancies (V_C), has been a major cause of device failures like low field effect mobility.

José Coutinho and Vitor Torres from the Theoretical and Computational Physics group at the I3N-UA, employed quantum-mechanics within hybrid density functional theory, to unveil the optical, electronic and magnetic properties of the VC defect in 4H-SiC [2]. They found that VC exhibits a rich catalog of atomistic structures that depend on the sublattice site, charge state, crystal-field effects, and more importantly a pseudo-Jahn-Teller effect. The latter solves a long-standing argument regarding the assignment and identification of the V_C defect in 4H-SiC. As observed by electron-paramagnetic resonance [3], the defect adopts a distorted structure, despite the lack of an explanation for such distortion. José Coutinho and Vitor Torres found out that the pseudo-Jahn-Teller effect in V_C dramatically lowers the energy of the defect by changing the local bonding, accounting well for the observations (see Figure).

The resulting model is also able to explain the observed inverted order of ionization energies related to the defect. The VC defect is able to capture two electrons. For the double-minus charge state, thermal emission of the first electron immediately induces a second emission. The research carried by the authors was able to explain this phenomenon on the basis of an exchange between Coulomb repulsion between electrons and chemical bonding due to the pseudo-Jahn-Teller effect.