**CT9** PHYSICS, CHEMISTRY AND MATERIALS PROPERTIES | **JOLIOT-CURIE & OCCIGEN: 6.2 MILLION HOURS**

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**BIOLOGY, CHEMISTRY AND MATERIALS**

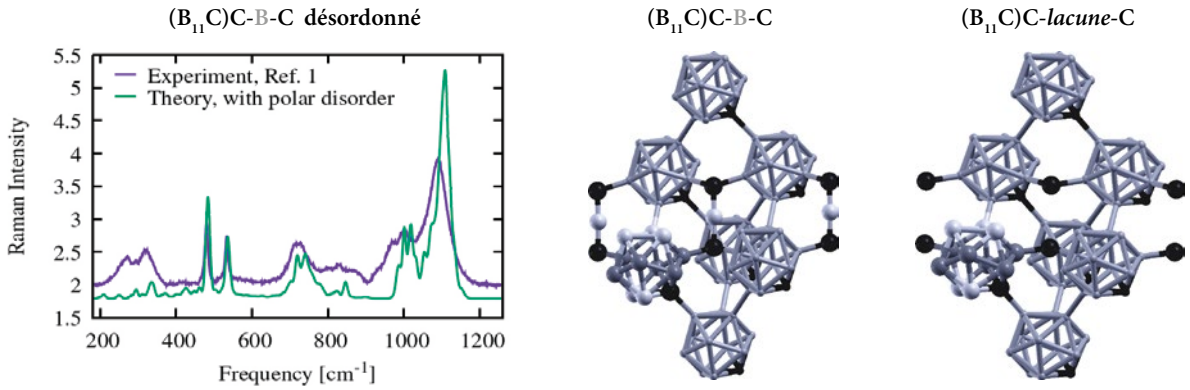
# Predicting the physical properties of materials

Our field of research is theoretical and numerical physics for materials science, and consists in the *ab initio* study of physical properties of materials, mainly with quantum-scaled methods based on the density functional theory (DFT). The latter enables us to reduce the complexity of the Schrödinger equation by using the theorem according to which the properties of the electronic ground state of a system of atoms and their electrons are determined uniquely by the electronic density of the ground state.

DFT calculations are performed without adjustable parameters, which has made it possible to predict with success and reliability the physical properties of many materials with controllable accuracy. An example is given *(figure on the left)* for B4C boron carbide, one of the hardest ceramics which is used for shielding military equipment and protecting people (bullet-proof vests). $B_4C$ is also an excellent neutron absorber useful for controlling the chain reaction in future fast neutron reactors.

For this material, we had theoretically predicted that the least energetic vacancy-based point defect is the ejection of the boron B atom from the C-B-C chain *(center figure)*, yielding C-vacancy-C configurations *(right figure)* which weaken the mechanical strength of $B_4C$. A series of experiments conducted at the Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC, Paris), using the very recent Paris-Edinburgh press with rotating anvil for tomography (RoToPEC), allowed to apply a torsional deformation to boron carbide, driving it in a controlled way into the plastic regime.

The damage have then been analysed by synchrotron X-ray diffraction and Raman spectroscopy, and interpreted using our DFT calculations. New peaks appearing in the two characterization methods turn out to be fingerprints of boron vacancies in the chains, in agreement with the theoretical prediction. This recent result confirms some of the ideas to strengthen $B_4C$ that are actively pursued with our partners from the IMPMC, the Institut de Recherche sur les CERamiques (IRCER, Limoges), and the Institut de Chimie de la Matière Condensée de Bordeaux (ICMCB).




Example of Raman spectrum computed within the density functional theory (left figure) of boron carbide, modelling the substitutional disorder of carbon atoms in polar sites of the B11C icosahedra by a supercell containing 405 atoms (blue line), compared with the experiment (violet line) [Credit: Physical Review Materials, 6 (2022) 016602]. Atomic structure of boron carbide in the ground state (center figure) and after plastic deformation (right figure [Credit: Acta Materialia, 226 (2022) 117553].