

Institut de Minéralogie et de Physique des Milieux Condensés
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SÉMINAIRE

Lundi 9 décembre, 10h30

*Salle de conférence, 4ème étage, Tour 22-23
IMPMC, Université P. et M. Curie, 4, Place Jussieu, 75005 Paris*

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ENERGY FRONTIER RESEARCH USING HIGH-PRESSURE: PREDICTION AND SYNTHESIS

Energy Frontier Research aiming at design, synthesis, and manufacture with higher performance and functionality, requires scientific innovative observations far beyond incremental advances in current energy technologies. Traditionally, basic science has relied on two variables or dimensions (namely temperature and composition) of known materials to understand underlying physics. Pressure is regarded as an entirely new dimension of science, which enables us to explore much broader range of thermo-mechanical conditions by accessing extreme states of matter. In this presentation, I will show recent progress on our theory-experiment collaborative works in this direction. Crystal structure searching using density functional theory predicts possible novel phases and guides our experiments. I will present our recent successful examples. Especially, I will show our recent discovery of a new silicon allotrope which is stabilized at ambient conditions. Interestingly, it possesses a quasi-direct band-gap with ~ 1.3 eV, which is the optimal band-gap for photovoltaic applications.