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Abstract for an Invited Paper for the SHOCK13 Meeting of the American Physical Society

Jamieson Award Talk - Novel Materials Prediction and Experimental Synthesis under Pressure DUCKYOUNG KIM, Carnegie Institute Washington

Pressure enables us to explore entire new dimension of materials science by perturbing energy landscape of materials beyond conventional thermodynamics limits. Realization of novel functional energy materials, synthesized under pressure, to ambient conditions can provide another insight to solve current Energy Challenge. 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. Experimental observations provide inputs for refinement of calculations. I will present our recent successful examples to highlight the importance of integrated experiment-theory collaboration for Energy Frontier Research.