

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Novel sp³-hybridized framework structure of group 14 elements
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Ames Lab, US DOE — Using genetic algorithm atomic structure prediction method
and first-principles calculations, we discovered a novel low-energy metastable structure
of group 14 elements in P42/mnm symmetry. The P42/mnm structure is a
cage-like distorted sp³-hybridized framework structure with the cage's volume \sim
4% larger than the average cage's volume of the clathrate type-I structure, indicating
P42/mnm structure a good gases or metal atoms encapsulation structure. The
band structure calculations show that P42/mnm Si and Ge are semiconducting with
energy band gaps close to the optimal values for optoelectronic or photovoltaic applications.
The metal atom encapsulation P42/mnm structure of group 14 elements
could also be a candidate for rattling-mediated superconducting or “a phonon glass
and an electrical crystal” thermoelectric materials.

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Date submitted: 15 Nov 2013

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