Density-functional-theory study of the Ga split-interstitial in GaAs

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- Density-functional theory (DFT) was used to study the C_{2v} 110g Ga interstitial in GaAs (see inset).
- DFT formation energies were analyzed using a new *bounds-analysis approach*,[1] and structural stabilities were evaluated using the dimer method.[2]
- Since the −1/−2 levels coincide with the upper bound, the −2 charge state is a delocalized conduction-band state (and thus not a Ga interstitial state).
- The C_{2v} structure is unstable in the 0, +1, and +2 charge states, so the +1/0, and +2/+1 levels will not be relevant to QASPR modeling.
- However, the 0 state is relevant to QASPR modeling since the −1 state transforms upon capturing a hole.

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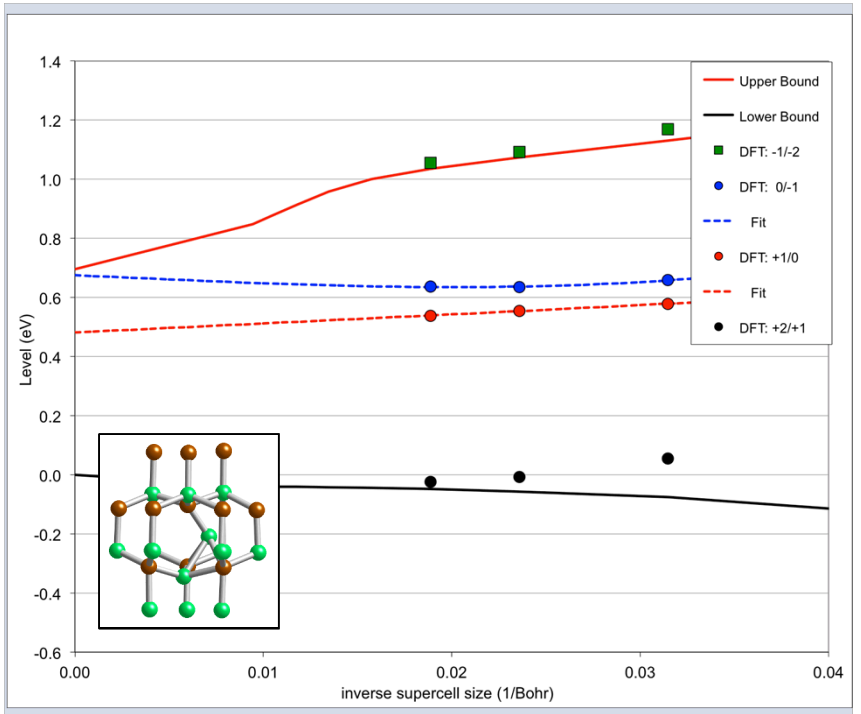
Platform/Campaign: Cielo/CCC-6
Usage: 1.39 days

Bounds analysis of the C_{2v} 110g Ga interstitial



[1] N. A. Modine, A. F. Wright, and S. R. Lee, Computationl Materials Science, **92**, 431 (2014).
[2] G. Henkelman and H. Jonsson, Journal of Chemical Physics, **111**, 7010 (1999).
[3] E. Burstein, Phys. Rev. **93**, 632 (1954); T. S. Moss, Proc. Phys. Soc. B **67**, 775 (1954).

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