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Relative stability of boron fullerenes: A dispersion-corrected density-functional study LARRY RICHE, ROSI GUNASINGHE, XIAO-QIAN WANG, Clark Atlanta University — We have studied the stability of various boron fullerene structures via dispersion-corrected desity-functional calculations. Our results reveal that the energy order of fullerenes strongly depends on the exchange-correlation functional employed in the calculation. A systematic study elucidates the importance of incorporating dispersion forces to account for the intricate interplay of two and three centered bonding in boron nano-structures. Futhermore, the inclusion of dispersion correction stabilizes high symmetry conformations that are vibrationaly unstable in the preceding density-functional calculations. We also discuss the use of graphics unit processor accelerated algorithms for the calculations.

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