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Unique stability of neutral interstitial hydrogen in cubic BN and diamond[1] JOHN L. LYONS, Center for Functional Nanomaterials, Brookhaven National Laboratory, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — In virtually all semiconductors and insulators, hydrogen interstitial impurities act as negative-U centers, implying that hydrogen is never stable in the neutral charge state. Using hybrid density functional calculations, which are crucial for obtaining accurate properties of defects in semiconductors, we find a different behavior for hydrogen interstitials in diamond and cubic BN. In diamond, we find that hydrogen is a very strong positive-U center, and the neutral charge state of the interstitial is stable over a Fermi-level range of more than 2 eV. In cubic BN, a III-V compound semiconductor with properties similar to diamond, we also find positive-U behavior, though over a much smaller Fermi-level range. We will discuss the electronic-structure origins of this negative-U behavior, and compare with the properties of hydrogen in other materials.

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