Supporting Information

How to Make Inert Boron Nitride Nanosheet Active for the Immobilization of Polysulfides for Lithium-Sulfur Batteries: A Computational Study

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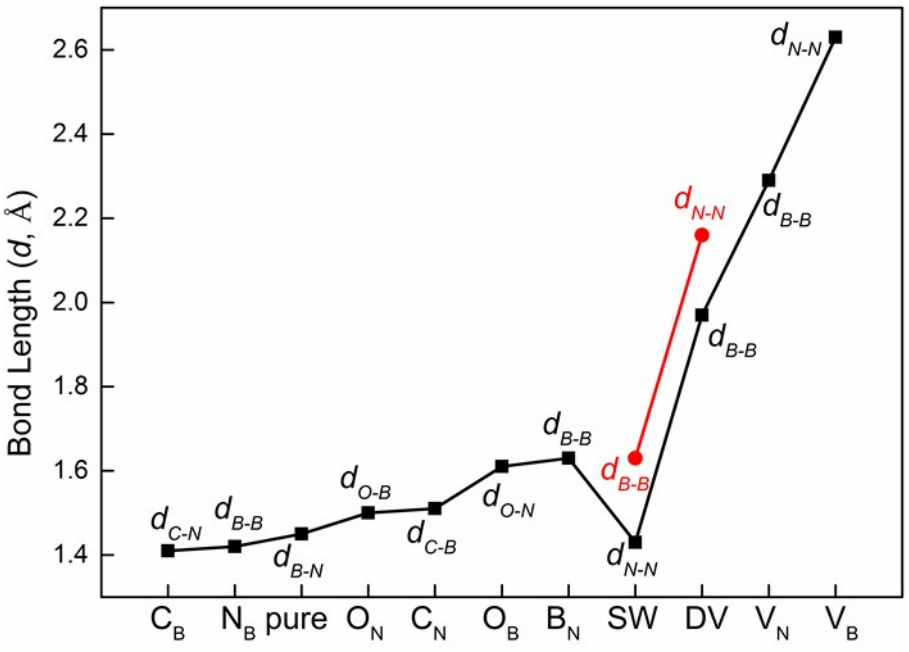

Fig. S1. Structural parameters of pristine, doped, and defective BN nanosheets.

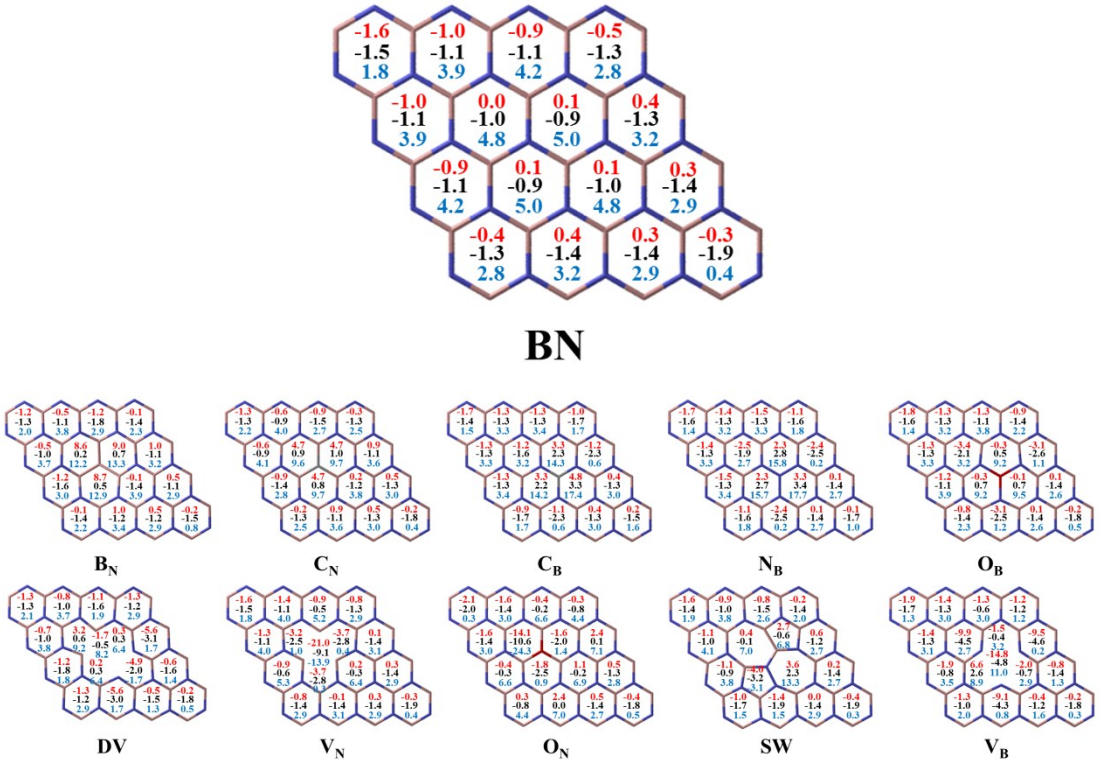

Fig. S2. Calculated nucleus independent chemical shift (NICS) values (ppm) at the ring centers (red), 1 Å above the ring centers (black) and their perpendicular tensors (blue) of various BN nanosheets. The NICS calculations were carried out at the PBE/6-31G* level of theory in Gaussian 09,[S1] and a finite nanoflake with the edge passivated by hydrogen atoms (not shown) is used for each model.

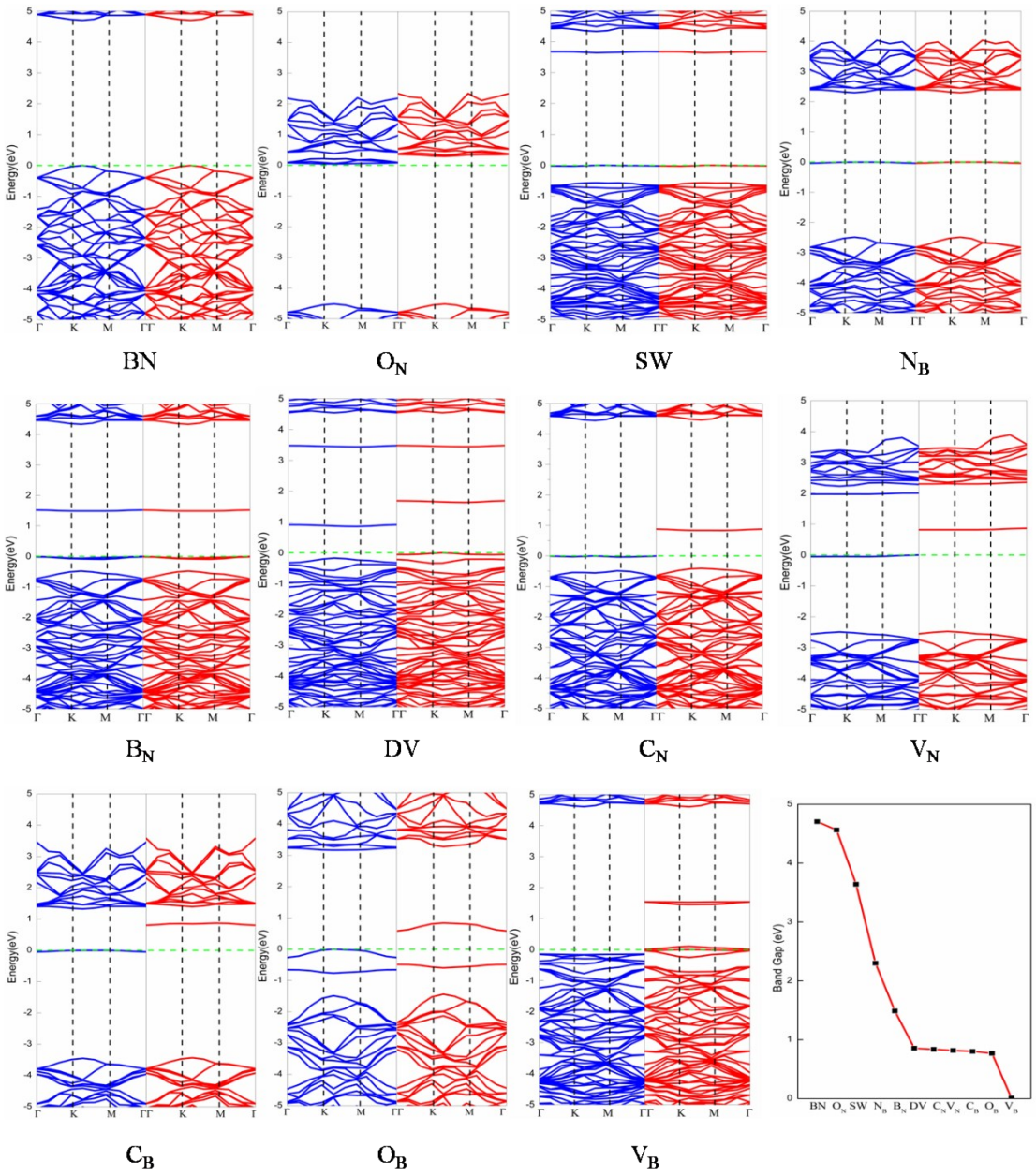

Fig. S3. The calculated band structures and band gaps of various BN nanosheets.

[S1] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci and G. A. Petersson, et al., Gaussian, Inc., Wallingford CT, 2010.