

## Correction to Boron Nitride Nanoribbons Become Metallic

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### Supporting Information

In the first paragraph under Table 1 in the original Letter (*Nano Lett.* **2011**, *11* (8), 3267–3273), an error was found related to the statement “No distortion due to Peierls-like instability toward the formation of oxygen dimers or trimers along the edges is observed when the number of unit cells in the supercell is increased to  $n = 2$  or  $n = 3$ ”. Indeed, for the O edge-terminated zigzag boron nitride nanoribbon (zBNNR), an O–O dimerization exists on the B edge and the O@B atomic wire becomes insulating due to this dimerization. Nevertheless, the zBNNR is still magnetic and metallic along the O@N atomic wire where the O atoms remain equidistantly separated. This dimerized structure is in fact more stable than the undistorted structure, and therefore it represents the global minimum structure of the ribbon. Using a narrower O-[BN]<sub>8</sub>-O(2) ribbon as an example, the dimerization energetics and the electronic structure of the dimerized structure are discussed in the new Supporting Information file. This finding does not affect our conclusion that, with O ribbon edge terminations, the zBNNRs become metallic. The results of the other functionalization scenarios presented in the paper are not affected.

### ASSOCIATED CONTENT

#### Supporting Information

Potential energy surfaces as a function of O–O distance alternation on the B and N edges, spin-polarized band structure, PDoS, and TDoS of the dimerized O-[BN]<sub>8</sub>-O(2). This material is available free of charge via the Internet at <http://pubs.acs.org>.

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