Supporting Information

Evolutionary Structure Prediction of Two-dimensional IrB₁₄:

A Promising Gas Sensor Material

Jun Yu^{#, 1}, Mohammad Khazaei^{#, 2}, Naoto Umezawa^{2, 3}, Junjie Wang^{*, 2, 4}

¹Advanced Manufacturing Research Institute, National Institute of Advanced Industrial Science and Technology, 1-2-1 Namiki, Tsukuba, Ibaraki, Japan.

² International Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan.

³ Samsung Electronics, Semiconductor R&D Center, 1, Samsungjeonja-ro, Hwaseong-si, Gyeonggido 18448, Korea

⁴ Materials Research Center for Element Strategy, Tokyo Institute of Technology, 4259 Nagatsutacho, Midori-ku, Yokohama, Kanagawa 226-8503, Japan.

[#] These authors contributed equally.

Email: wang.junjie0810@gmail.com



Figure S1. Convergence test of k-mesh.



Figure S2. Calculated phonon band structures for 2D-IrB₁₄(a), 2D-IrB₈ (b), 2D-IrB₁₀ (c), 2D-IrB₁₂ (d) and 2D-IrB₁₆ (e). Phonon density of states (DOS) of 2D-IrB₁₄ is also shown in (a).



Figure S3. The final configurations of 2D IrB_{14} (with CO adsorbed) after 4500 fs FPMD simulations at 500K, 1000K, 1500K and 2000 K.



Figure S4. Calculated IR spectra of CO molecule on 2D-IrB₁₄ plotted in comparison with that of free CO molecule.