Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

Graphene quantum dots embedded in a hexagonal BN sheet: Identical influences of zigzag/armchair edges

Ruiqi Zhao,[a,b,c] Jinying Wang,[a,b] Mingmei Yang, [a,b] Zhongfan Liu,*[a,b] and Zhirong Liu*[a,b]

[a] *College of Chemistry and Molecular Engineering, Peking University, Beijing, 100871, China.*

E-mail: zfliu@pku.edu.cn (Zhongfan Liu), LiuZhiRong@pku.edu.cn (Zhirong Liu).

[b] *Center for Nanochemistry, State Key Laboratory for Structural Chemistry of Unstable and Stable Species, and Beijing National Laboratory for Molecular Sciences (BNLMS), Peking University, Beijing 100871, China*

[c] *College of Physics and Chemistry, Henan Polytechnic University, Henan 454003, China*

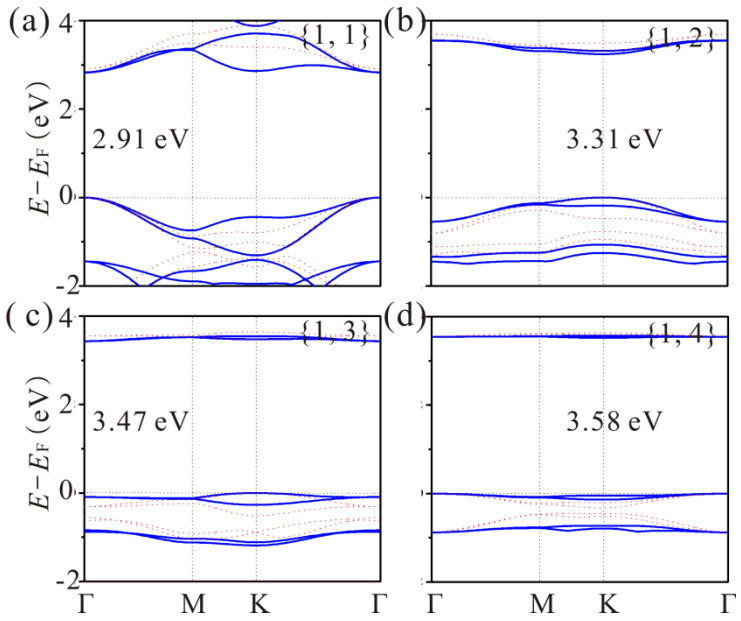

Fig. S1 Energy band structures for ZHR- GQDs embedded in BN with a system notation {*R*, *W*} of (a) {1, 1}, (b) {1, 2}, (c) {1, 3} and (d) {1, 4} obtained from TB (blue solid lines) and DFT (red dashed lines). The value obtained from TB is also labeled in each panel.

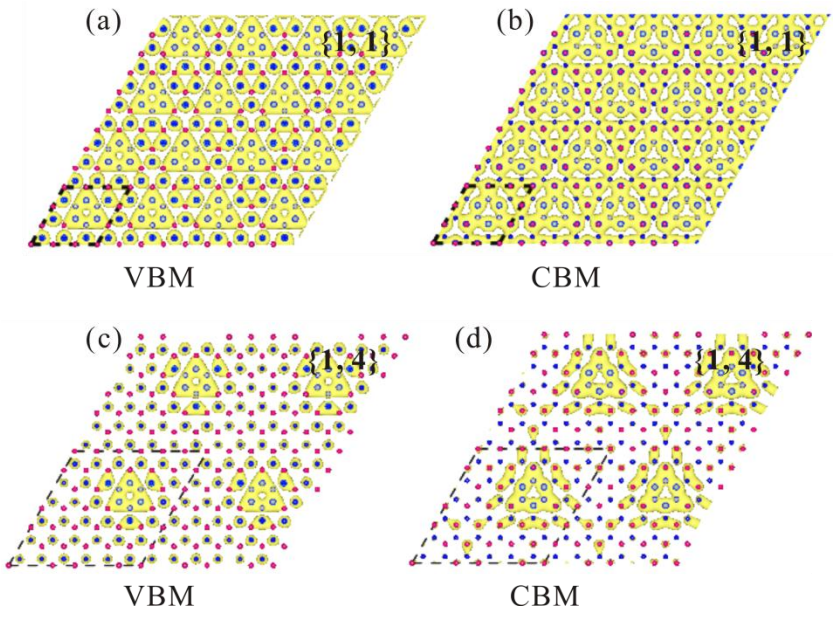

Fig. S3 The electron charge density distribution of the valence states of ZHR- GQDs in BN at the Γ point with different {*R*, *W*} (isosurfaces correspond to the value of 5×10^{-4} eÅ^{-3}). (a) VBM of {1, 1}, (b) CBM of {1, 1}, (c) VBM of {1, 4}, and (d) CBM of {1, 4}. The supercell is also labeled by dashed rectangle in each panel. The red (dark gray), blue (black), and gray (light gray) spheres represent B, N, and C atoms, respectively.