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Origin of trion fluorescence in WS₂ monolayer edges

For the CVD-grown TMDs, PL enhancement at edges and grain boundaries is a quite common phenomenon, even many research efforts have concentrated on this issue [1-4], the physics fundamental behind remains unknown. We use the density functional theory to study the electric properties of the edges of WS₂ monolayer and PL enhancement at edges. We show that oxygen introduction to edges creates the oxygen terminated zigzag W-edge which may be the origin of n-doping and trion-dominated fluorescence in WS₂ monolayer edge. In addition, the metallic behavior disappears, a n-doping semiconducting behavior occurs instead. Because of the n-doping in the area close to the edge, more negative trions will form under the excitation of external radiation, and giving rise to the trion fluorescence in WS₂ monolayer edges.

References

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Figures

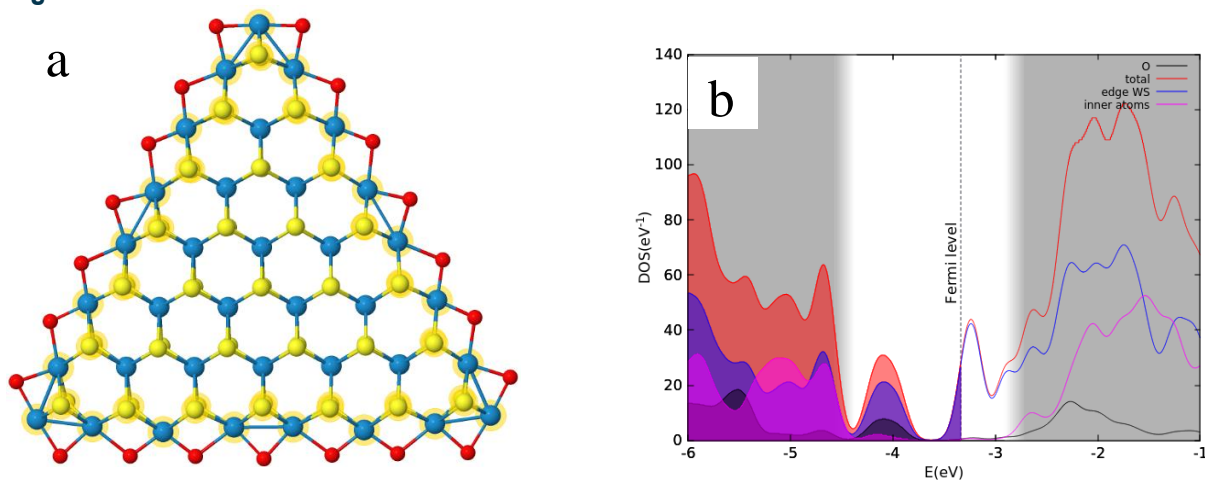


Figure 1: (a) Top view of triangle-shaped WS₂ with and without oxygen adsorbed after DEF relaxation. Shaded spheres denote the edge W and S atoms. (b) DOS of triangle-shaped WS₂ with and without oxygen adsorbed.