Supporting Information

Vastly Enhancing the Chemical Stability of Phosphorene by Employing

Electrical Field

Junfeng Gao, Gang Zhang* and Yong-Wei Zhang†

Institute of High Performance Computing, A*STAR, Singapore, 138632, Singapore

^{*} zhangg@ihpc.a-star.edu.sg

[†] zhangyw@ihpc.a-star.edu.sg



Figure S1. The charge transfer between O_2 and phosphorene: the O_2 molecule physisorbed on freestanding phosphorene (a) and on phosphorene with $MoSe_2$ substrate (b); the O_2 molecule chemisorbed on freestanding phosphorene (c) and on phosphorene with $MoSe_2$ substrate (d). ρ is the plane-averaged differential charge density and ΔQ is the amount of transferred charge along the z direction, respectively.



Figure S2. The band structure of O_2 physically adsorbed on phosphorene with MoSe₂ substrate under various electric fields: a) 0.0 V/Å, b) 0.2 V/Å, c) 0.3 V/Å, and d) 0.6 V/Å. Red, green and yellow shades on the lines represent the charge contributions of O_2 , phosphorene, and MoSe₂ to each band, respectively. The partial density of states of O, P, Mo and Se atoms corresponding to the band structures above: e) 0.0 V/Å, f) 0.2 V/Å, g) 0.3 V/Å, and h) 0.6 V/Å.



Figure S3. Determination of peaks of partial DOS for O_2 physically adsorbed on phosphorene with MoSe₂ substrate under a -0.3 V/Å electric field. The hidden peaks of DOS are revealed by the second derivative of DOS.