

Supporting Information for:

Exploring the Nature of Interaction and Stability between Water-Soluble Arsenic Pollutants and Metal-Phosphorene Hybrids: A DFT Study

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S1. Density of State plots

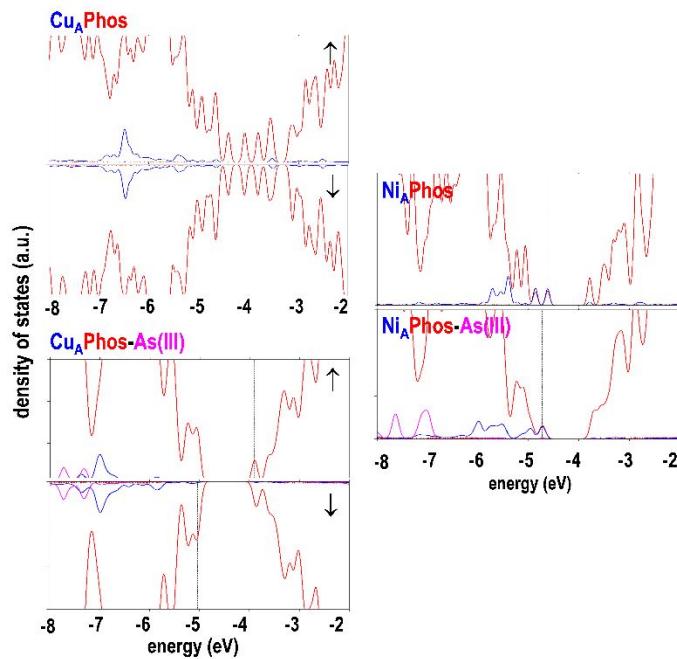


Fig. S1. Partial density of states (DOS) plots of the $\text{M}_\text{A} \text{Phos-As(III)}$ systems. Blue, red and pink lines correspond to the states coming from the metal, phosphorene, and As(III), respectively. The vertical dotted line indicates the position of the HOMO level.

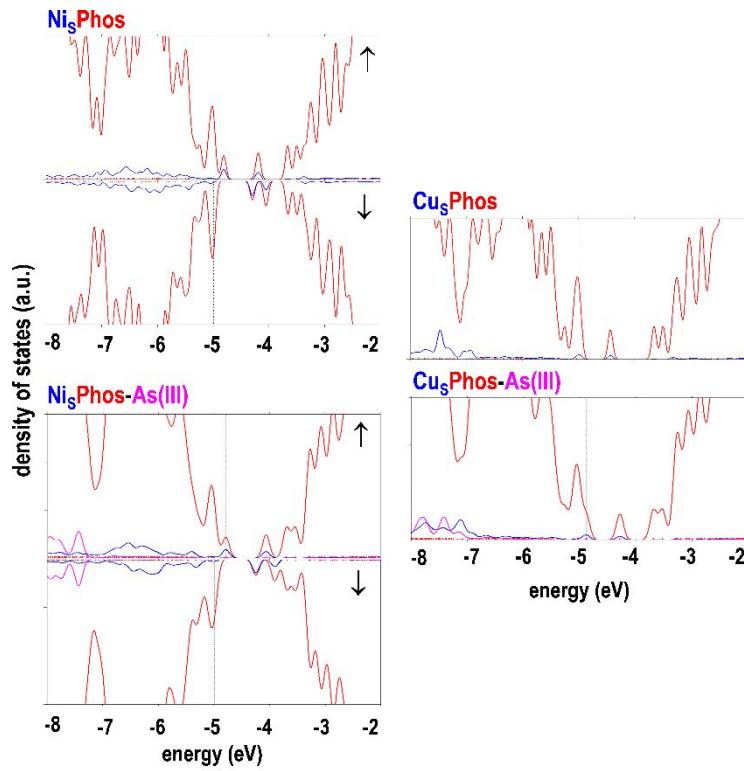


Fig. S2. Partial density of states (DOS) plots of the M_SPhos-As(III) systems. Blue, red and pink lines correspond to the states coming from the metal, phosphorene, and As(III), respectively. The vertical dotted line indicates the position of the HOMO level.