Dataset on 2D Material-Metal Interfaces: Adhesion, PES Corrugation, Interface Distance, and Supercell Area

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Data Records

This dataset presents the computed energetic properties of a 2D-material-metal interfaces. It includes adhesion energies, potential energy surface (PES), equilibrium interface distances and the supercell areas, that were obtained in an automatized way using TribChem software [1]. The dataset contains Graphene and six transition-metal dichalcogenides TMDs (MoS_2, $MoSe_2$, $MoTe_2$, WS_2, WSe_2, and WTe_2) interfaced with fourteen metals. All data generated in this work are available in the excel sheet uploaded.

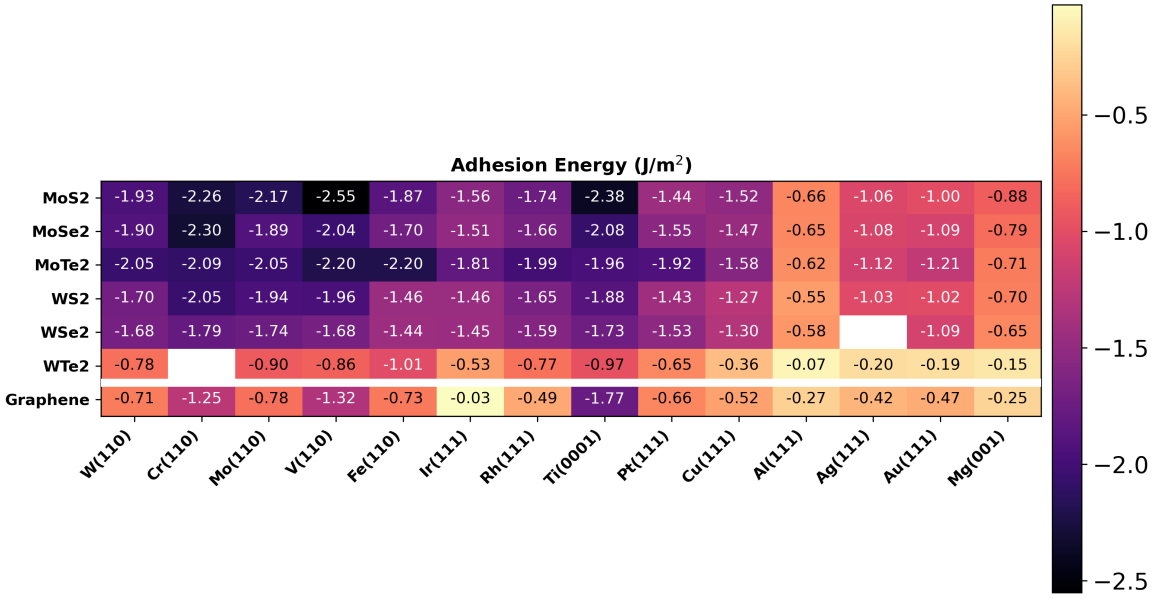

Figure 1: Adhesion energies obtained for all investigated 2D/metal interfaces. Each cell represents one interface, 2D materials are the rows, and metals are the columns, darker colors indicate stronger adhesion (more negatives). Among the 2D materials, TMDs generally adhere more strongly than graphene. The voids in this Figure and others namely WSe_2-Ag(111) and WTe_2-Cr(110) are interfaces that Zur algorithm didn't find the match within the allowed strain and maximum supercell area.

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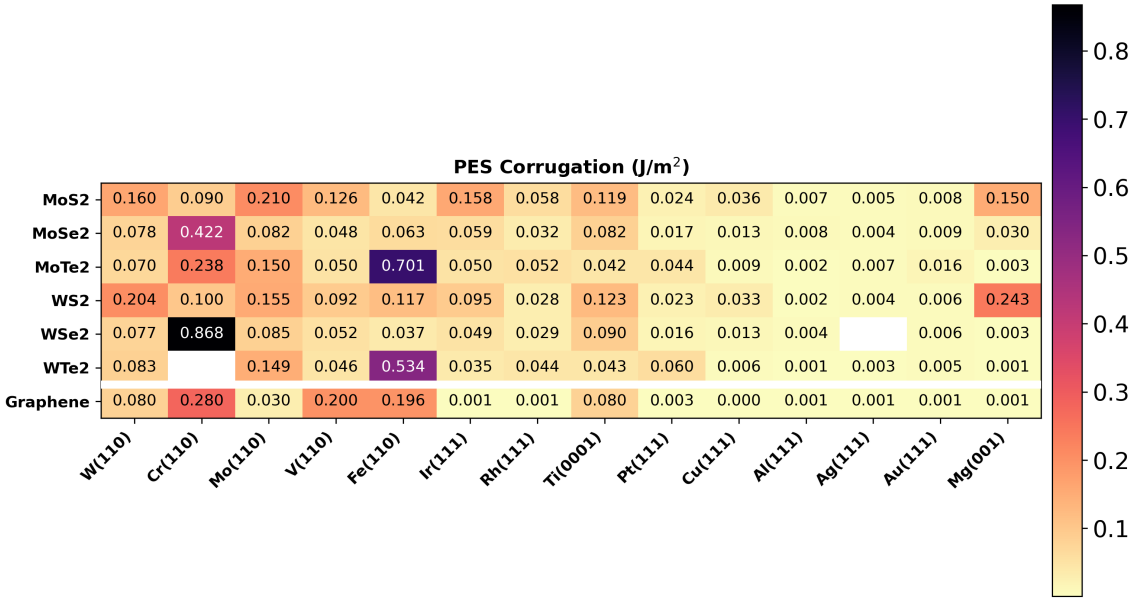

Figure 2: PES values for the investigated 2D material/metal interfaces. Darker colors show higher PES corrugation. It can be seen that most interfaces exhibit relatively small corrugation values, typically below 0.1 J/m^{-2}. However, certain interfaces such as 2D-Fe(110) and 2D-Cr(110) show higher corrugation energies. The highest average PES corrugation among the investigated interfaces corresponds to $MoTe_2$-metal interfaces, with a value of approximately 0.10245 J/m^2, whereas the lowest average is observed for WSe_2-metal interfaces around 0.0421 J/m^2.

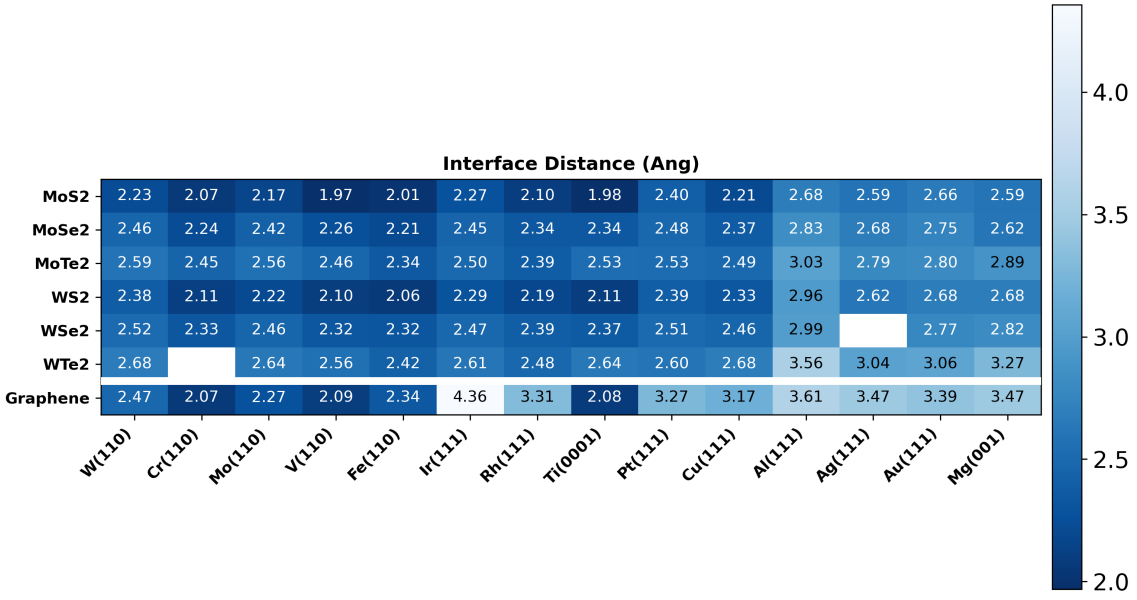

Figure 3: Equilibrium distance (in Å) between the surface atomic layers of the metals and of the 2D material after structural relaxation. Darker colors correspond to a smaller interface distance.

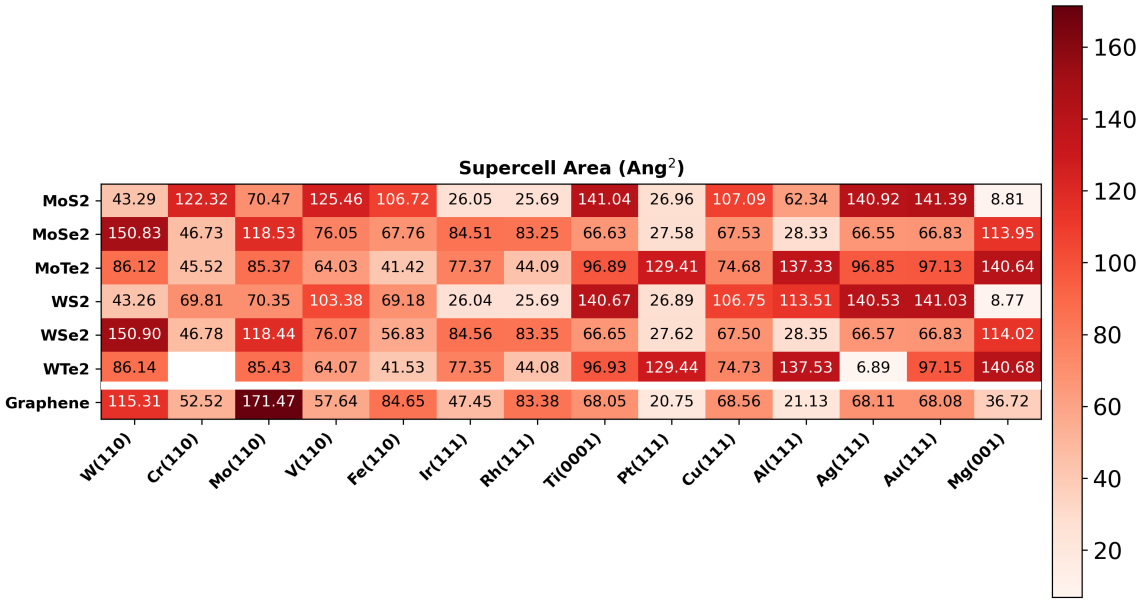

Figure 4: Lateral supercell areas used for constructing each 2D/metal interface. The supercell area (in Å^2) represents the in-plane surface area of the interface model after lattice matching between the 2D material and the metallic substrate. Darker colors correspond to large supercell area.

Acknowledgments

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References

[1] G. Losi, O. Chehaimi, and M. C. Righi. "TribChem: A Software for the First-Principles, High-Throughput Study of Solid Interfaces and Their Tribological Properties". In: *Journal of Chemical Theory and Computation* 19.15 (2023), pp. 5231–5241. DOI: 10.1021/acs.jctc.3c00459.