

Atomic adsorption on graphene from first principles: influences of defects and dispersion interactions

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This study presents a comprehensive analysis of atomic adsorption on graphene, focusing on pristine and defective graphene structures using Density Functional Theory (DFT). We compiled a complete database of atomic adsorption energies for elements up to atomic number 86 on pristine graphene, calculated using projector augmented wave (PAW) methods and dispersion corrections like PBE+D2, PBE+D3, and vdW-DF2. Significant findings include the importance of dispersion interactions, especially for elements with low atomic weights and high cohesive energies. Additionally, we explored the impact of single vacancies and Stone-Wales (SW) defects on graphene's chemical reactivity. We observed enhanced binding at vacancies, with elements higher in cohesive energy showing stronger bonds, suggesting that defect engineering could tailor graphene's properties for advanced applications. Furthermore, the SW defect not only increased adsorption strength but also, under mechanical deformation, led to significant reorganization within the graphene structure, impacting its reactivity and potential utility in materials science. This comprehensive analysis underscores the nuanced interplay of atomic structure, defects, and adsorbate characteristics in defining the properties of graphene, revealing ways for its optimized use in technology and material science.

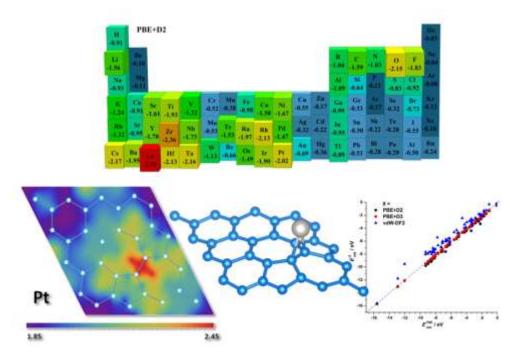


Figure 1. Adsorption energy of the elements of PTE on pristine graphene (top), heatmap of Pt adsorption on SW-graphene (bottom, left) and a structural model of the most stable adsorption configuration (bottom, center), correlation of adsorption energy for different computational schemes on monovacant graphene (bottom, left)

Acknowledgement: I.A.P, A.S.D and A.Z.J acknowledge the support provided by the Serbian Ministry Science, Technological Development, and Innovation (451-03-65/2024-03/200146). The computations and data handling were enabled by resources provided by the National Academic Infrastructure for Supercomputing in Sweden (NAISS) at the NSC center of Linköping University, partially funded by the Swedish Research Council through grant agreements no. 2022-06725 and no. 2018-05973.