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Effect of single-layer MoS_2 support on the geometry and electronic structure of transition metal nanoparticles[1] TAKAT B. RAWAL, DUY LE, TALAT S. RAHMAN, Department of Physics, University of Central Florida — We present results of density functional theory based calculations of the geometry and electronic structure of small (29-atom) transition (TM) nanoparticles (NPs) supported on single-layer MoS_2, with and without S-vacancy defects. Among the prototypes considered, the NPs bind more strongly on defect-laden rather than pristine MoS_2 – in the order Cu_{29}>Ag_{29}>Au_{29} for defect-laden and of Cu_{29}>Au_{29}>Ag_{29} for pristine. Interestingly, van der Waals interactions play a stronger role in the case of Au_{29} than in the other two. Strong interaction between the NPs and defect-laden MoS_2 is also facilitated by the close contact of their "boat-shape" with v-like-shape of single-layer MoS_2 formed when laden with S vacancies. We also find that the trend for the charge transfer from NPs to MoS_2, regardless of its form (pristine or defect-laden), is Cu_{29}>Ag_{29}>Au_{29} and that defect-laden MoS_2 donates more charge than its pristine counterpart does. Among all NPs, the largest shift of d-band center toward the Fermi level occurs in the case of defect-laden-supported Au_{29}. Our results suggest that defect-laden MoS_2 is good support for anchoring and for tuning electronic properties of TM NPs, which have potential in catalytic applications.

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Duy Le
Department of Physics, University of Central Florida

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