Post-synthesis Introduction of Transition Metal Impurity into Molybdenum Dichalcogenides - Density Functional Study

J. Karthikeyan[1] H. Komsa[1] M. Batzill[2] A. Krasheninnikov[1,3]

[1]Department of Applied Physics, Aalto University, P.O. Box 11100, 00076 Aalto, Finland
[2]Department of Physics, University of South Florida, Tampa, Florida 33620, United States
[3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Introduction of impurities into a material, conventionally during its growth, is one of the promising ways to tune electronic and magnetic properties of bulk and nanomaterials as well. However, in two-dimensional materials, the impurities can be directly incorporated by depositing dopant atom at an elevated temperature, as demonstrated for $MoTe_2$ layer[1,2]. We have employed density functional calculations to find which transition metals are readily embedded into molybdenum dichalcogenides, instead of trivial clustering on the surface. Further, we rationalize the energetics and induced magnetic moment through atomic radii and the number of (s+d) electrons of TM atoms. Our results are in agreement with the available experimental data and should further guide the experiment.

[1] Paula Mariel Coelho, Hannu-Pekka Komsa, Horacio Coy Diaz, Yujing Ma, Arkady V. Krasheninnikov, and Matthias Batzill, *ACS Nano* **12**, 3975-3984 (2018).
[2] Paula Mariel Coelho, Hannu-Pekka Komsa, Vijaysankar Kalappattil, Jeyakumar Karthikeyan, Kinga Lasek, Manh-Huong Phan, Arkady V Krasheninnikov, and Matthias Batzill, *Advanced Electronic Materials* Accepted (2019).