The Nanobots First-Year Undergraduate Research Experience Modeling TMDs with ReaxFF

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The Nanobots First-Year Undergraduate Research Experience involves chemistry students at a primarily undergraduate institution in materials science research during their first semester of college.

The pedagogical goal of the program is to provide students with the relevance, community, and mentoring to be successful in Introductory STEM courses. The impact of early research experiences on retention in STEM has long been recognized, but difficult to implement on a large scale. First-year student volunteers (10 during the Fall 2021 pilot, 8 continuing into Spring 2022, invited from two sections of General Chemistry) meet weekly to model the behavior of MoS_2 using the ReaxFF empirical force field technique as implemented in the Amsterdam Modelling Suite (AMS), as developed by the Software Chemistry & Materials (SCM) company. Preliminary findings suggest that this computational method is well suited to involvement of a large number of undergraduate students in research problems. Students have learned about the utility of transition metal dichalcogenides for energy applications and computational modeling. They have made intellectual connections between the modeling activities and their General Chemistry courses. Students coalesced into a close community where they supported one another and received support from an involved mentor.

The research goal of the program is to further develop the ability to model metal chalogenides and elucidate the role of vacancies in promoting ion exchange processes. Post-synthetic transformation of nanoscale TMDs is an important avenue for tuning properties. Despite several papers reporting the interchange of metals and chalcogenides via cation and anion exchange, this synthetic technique has not been broadly applied, nor is cation and anion exchange well understood in TMD systems. To better understand how to promote ion exchange in TMDs, we modeled the process of incorporating new sulfur atoms into MoS_2 with varying vacancy positions and concentrations.