DEEP LEARNING OF CVD GROWTH AND PHASE-TRANSITION PATHWAYS IN LAYERED MATERIALS

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Electrical and optoelectronic properties of two-dimensional (2D) transition metal dichalcogenides (TMDCs) can be tuned by exploiting their polymorphism. Here, polymorphism in TMDCs and their growth by chemical vapor deposition (CVD) are examined using deep generative models namely, the variational autoencoder (VAE) and Restricted Boltzmann Machine (RBM), trained with molecular dynamics (MD) simulation data. The VAE correctly identifies pathways connecting the semiconducting (2H) and metallic (1T) phases via novel intermediate structures called a and *b* in $MoWSe_2$ alloy. These intermediate structures are similar to those observed in a 2D MoS_2 by scanning transmission electron microscopy. Structures generated solely by VAE are combined to form novel $MoWSe_2$ devices with *a* and *b* interfaces. Quantum simulations based on density functional theory show that interfaces synthesized by VAE are stable and the devices with those interfaces are suitable for novel nanoelectronics applications. A novel deterministic RBM algorithm is used to identify 2H and 1T phases and defects in reactive MD simulations of the synthesis of a MoS_2 monolayer by CVD. Applications of the deterministic RBM approach to modeling of experimental data will also be presented.

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