

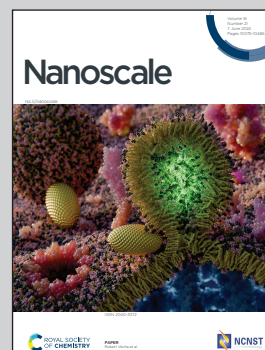


**Showcasing research from Prof. Terence Musho's group at West Virginia University, West Virginia, USA.**

**Autonomous generation of single photon emitting materials**

This image portrays a digitally-alchemical realm fostering efficiency amidst mystery in crafting molecular-based single-photon emitting materials. A SMILES language model was devised to generate synthetic datasets for AI exploration in quantum sensing, computing, and communication. Trained on a small experimental dataset, the model scales to millions, utilizing a unique sampling method to exceed training ranges and minimize bias. Chemical stability is ensured through a high-throughput semi-empirical quantum chemistry validation step. The source code is available on GitHub, while generated data can be accessed *via* the NOMAD materials science database.

**As featured in:**



See Robert Tempke and Terence Musho, *Nanoscale*, 2024, **16**, 10239.