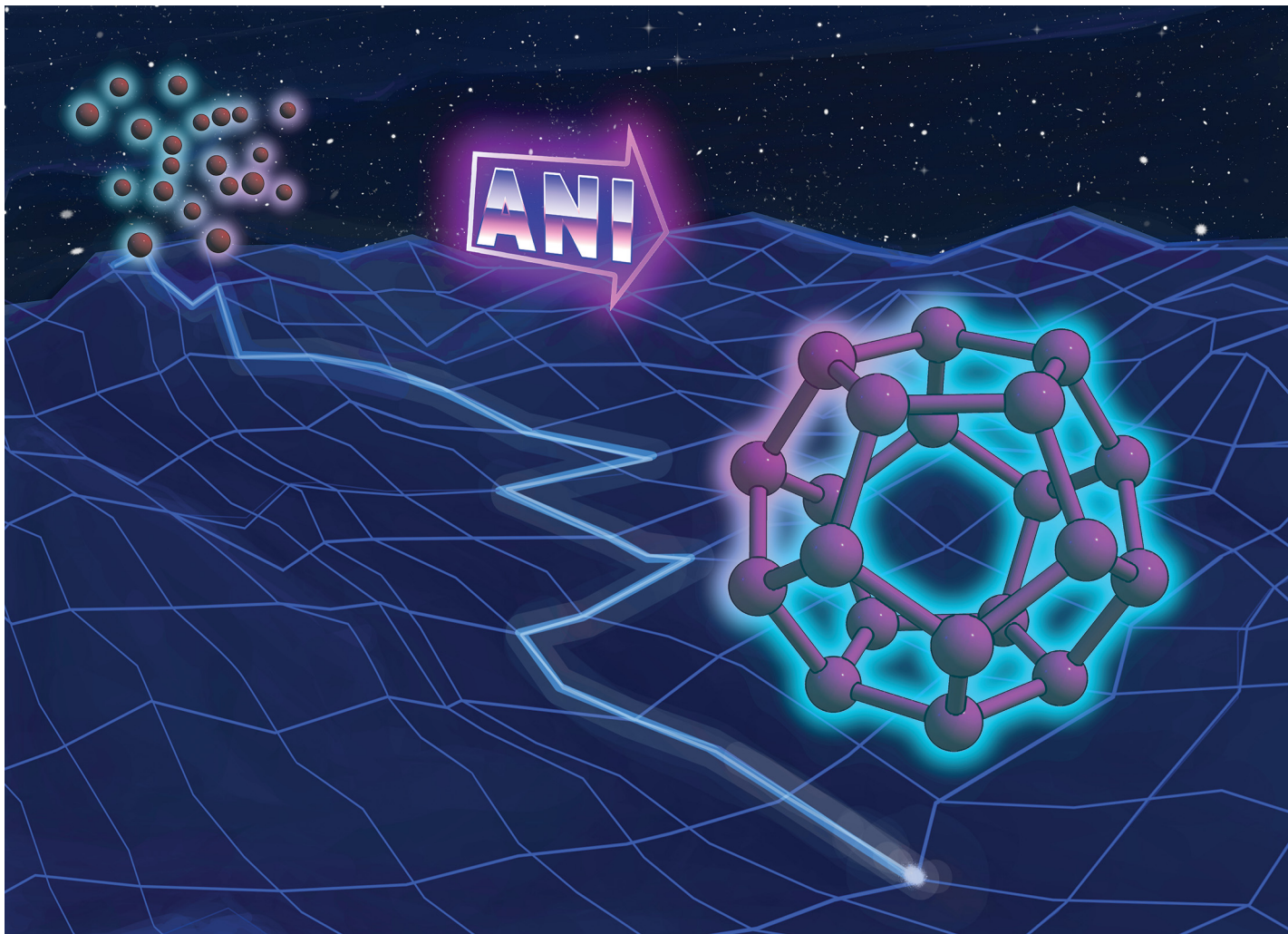


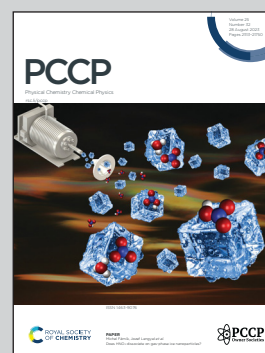


Research from the group of Prof. Alexander Boldyrev at Utah State University, and group of Dr Sergei Tretiak at Los Alamos National Laboratory, USA.

Neural network atomistic potentials for global energy minima search in carbon clusters

This work explores the application of neural network atomistic potentials, specifically ANI-1ccx and ANI-nr, for efficient global minima optimization in carbon clusters. We demonstrate that these potentials are robust PES pre-samplers, when combined with the cluster connectivity and distance restriction and subsequent DFT or *ab initio* calculations for structure and energy refinement.

As featured in:



See Nikolay V. Tkachenko, Anastasiia A. Tkachenko, Alexander I. Boldyrev *et al.*, *Phys. Chem. Chem. Phys.*, 2023, 25, 21173.