



Allocation: Illinois/135 Knh
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DETECTION OF AMINO ACIDS WITH HIGHLY SENSITIVE MoS₂ NANOPORES: TOWARD MACHINE LEARNING-BASED PREDICTIVE MODELS

Research Challenge

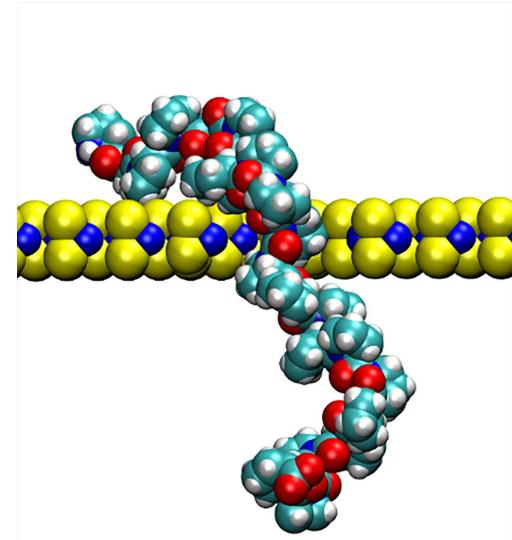
Designing biological and synthetic nanopores with predefined properties for molecular transport is one of the most challenging problems in biotechnology. Biological and synthetic nanopores have been employed for label-free, high-resolution sequencing of DNA. The challenges associated with identification of biological molecules using nanopores are the low signal-to-noise ratio, pore degradation, unique identification of individual molecular units in real time, and the high speed of molecular movement through a nanopore.

Methods & Codes

We performed Quantum Calculations based on VASP to determine interaction potentials and molecular dynamics simulations using LAMMPS to determine trajectories of amino acids. Each simulation box comprised of about 32,000 atoms contained a monolayer membrane of MoS₂, an amino acid chain, water molecules, and ions. The amino acid chain was pulled through a nanopore using an external force.

Why Blue Waters

We performed 4,103 molecular dynamics (MD) simulations of systems of up to 50,000 atoms and obtained 66 μs of molecular trajectories. Such expensive computations would not have been possible without a petascale supercomputer such as Blue Waters. LAMMPS, the MD package we use in our simulations, scales almost linearly with the number of cores on Blue Waters.



A snapshot of proline polypeptide translocation through the MoS₂ nanopore.

Results & Impact

We showed that a nanopore in an ultrathin MoS₂ membrane can be used to detect and identify all of the 20 standard amino acids in the translocating proteins. The high-precision, single-base resolution and fast biomolecular sequencing using nanopore technology can lead to the fabrication of inexpensive personal healthcare devices that will help provide targeted healthcare. This will enable predictive and personalized medicine and will mark a significant leap forward for clinical genomics and proteomics.