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Molecular Simulations of Polyamide Membrane Materials Used in Desalination and Water Reuse Applications: *Recent Developments and Future Prospects*

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Abbreviations used in this review:

Å	*Angstrom*
AFM	*atomic force microscopy*
AMBER	*Assisted Model Building and Energy Refinement;* R. Salomon-Ferrer,D.A. Case, R.C. Walker, An overview of the Amber biomolecular simulation package, WIREs Comput. Mol. Sci. 3 (2012) 198-210.
BSA	*Bovine serum albumin*
CA	*cellulose acetate*
CHARMM	*Chemistry at Harvard Molecular Mechanics, MD code; originally developed by Martin Karplus, Harvard University*
CN	*cellulose nitrate*
CNT	*carbon nanotube*
CVFF	*Consistent Valence Force Field;* P. Dauber-Osguthorpe, V.A. Roberts, D.J. Osguthorpe, J. Wolff, M. Genest, A.T. Hagler, Structure and energetics of ligand binding to proteins: E. coli dihydrofolate reductase-trimethoprim, a drug-receptor system, Proteins: Structure, Function and Genetics 4 (1988) 31-47.
GROMACS	*Groningen Molecular Simulation package*
LAMMPS	*Large-scale Atomic/Molecular Massively Parallel Simulator*
MD	*molecular dynamics*
MPa	*1 million Pascals ≈ 10 atm ≈ 150 psi*
MPD	*meta-phenylenediamine*
NAMD	*Nanoscale Molecular Dynamics MD code developed at Theoretical and Computational Biophysics Group at University of Illinois at Urbana–Champaign.*
NEMD	*Non-equilibrium molecular dynamics*
NF	*nanofiltration*
NMR	*nuclear magnetic resonance*
ns	*nanosecond*
OPLS-AA	*Optimized Potential for Liquid Simulations – All Atom;* W.L. Jorgensen, D.S. Maxwell, J. Tirado-Rives, Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids, J. Am. Chem. Soc. 118 (1996) 11225–11236.