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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 \approx 10 atm \approx 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.

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