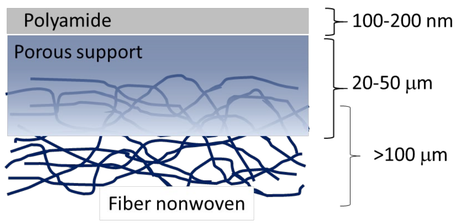
Carbon nanotube-aromatic polyamide nanocomposite membranes for micropollutants and boron rejection.

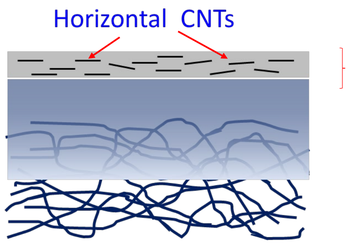
Rodolfo Cruz-Silva,[1] Ayaka Yamanaka[1,2], Haruka Takeuchi,[3] Hiroshi Ushiyama, Aaron Morelos,[1] Takuya Hayashi,[2] Kenji Takeuchi,[2] Syogo Tejima,[1,2] Mauricio Terrones,[1,4] Hiroaki Tanaka,[3] Morinobu Endo[1]

1 Research Initiative for Supra-Materials and Aqua Innovation Center, Shinshu University, Nagano, Japan.
2 Research Organization for Information Science and Technology, Nagano, Japan.
3 Research center for Environmental Quality Management, Kyoto University.
4 Department of Physics, Chemistry, Materials Science and Engineering, Center for 2-Dimensional and Layered Materials, and Center for Atomically Thin Multifunctional Materials (ATOMIC), The Pennsylvania State University, State College, PA,USA.

Typical polyamide thin film composite membrane

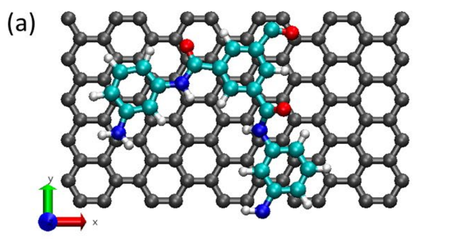


CNT-PA nanocomposite thin film membrane

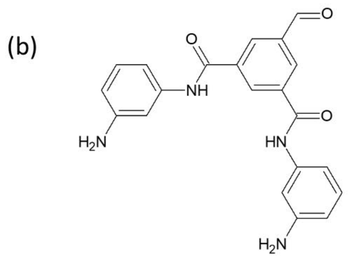


Membrane studied in this work

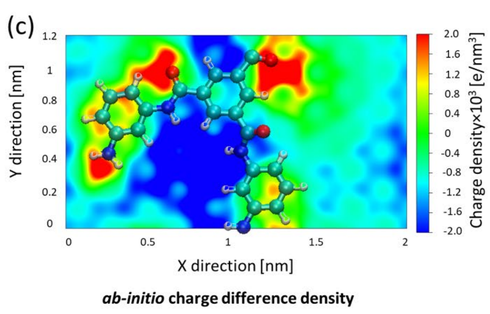
Charge calculation: ab initio vs QEq



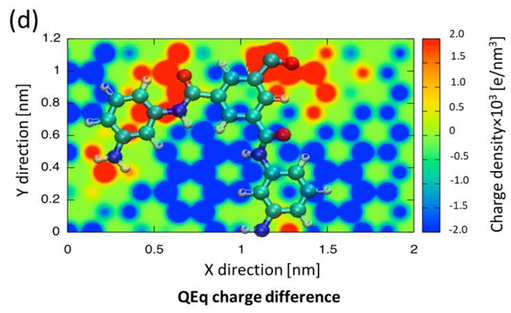
polyamide oligomer on graphene sheet



Model polyamide oligomer

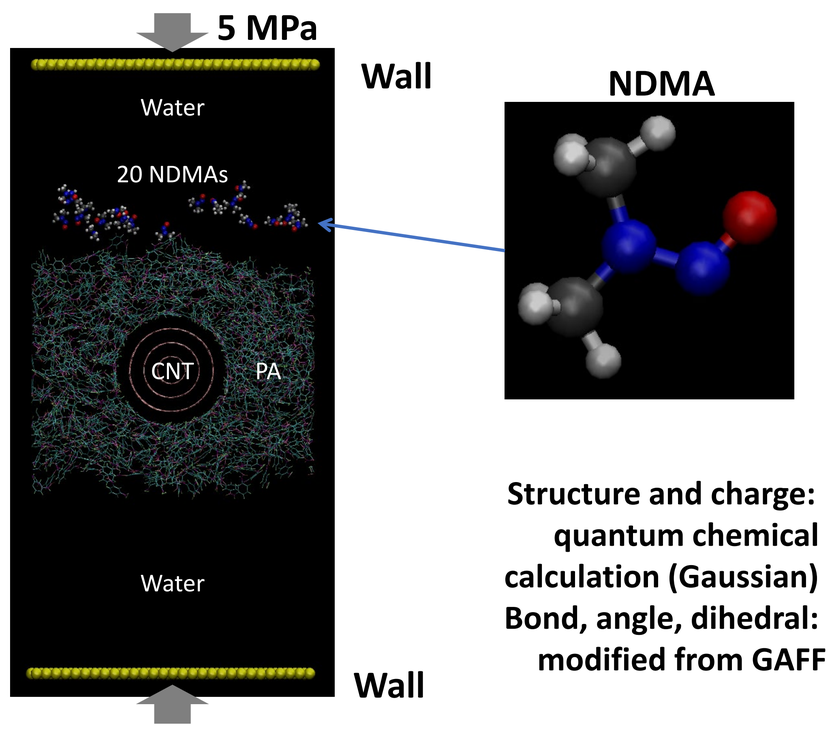


ab-initio charge difference density



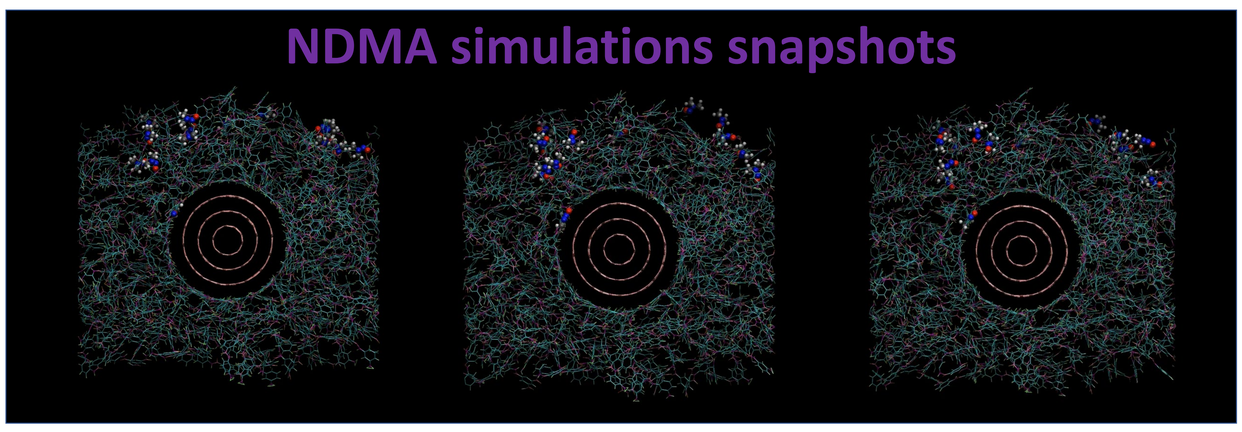
QEq charge difference

N-nitrosodimethylamine (NDMA) simulations

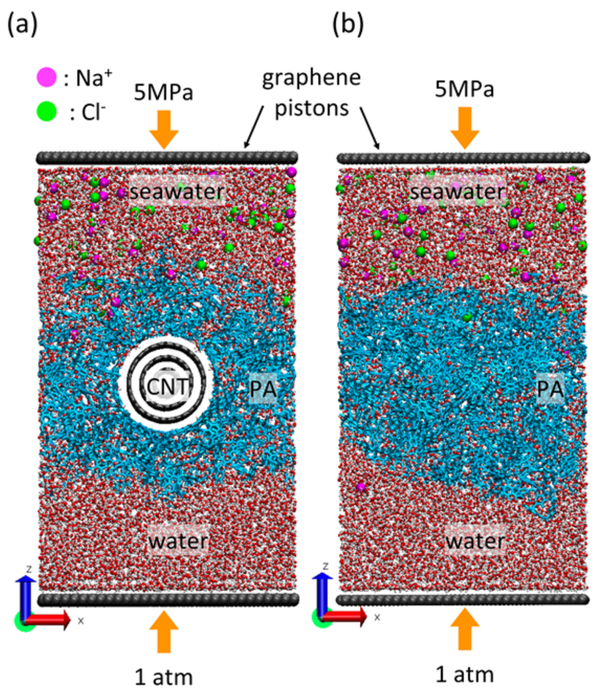


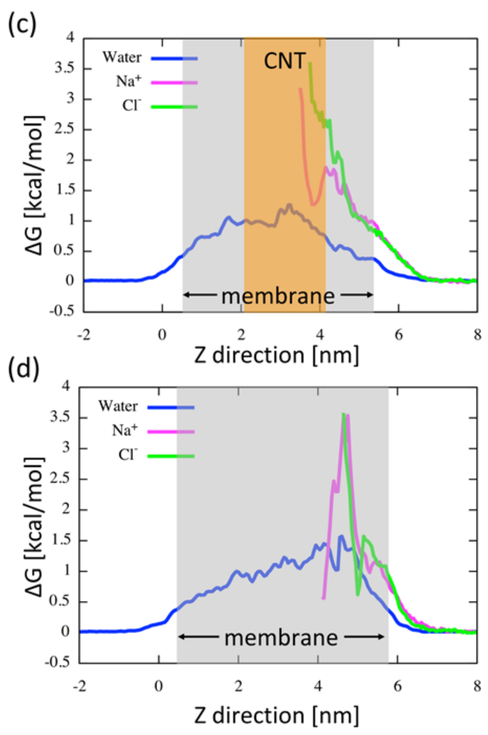
Structure and charge: quantum chemical calculation (Gaussian)
Bond, angle, dihedral: modified from GAFF

NDMA simulations snapshots

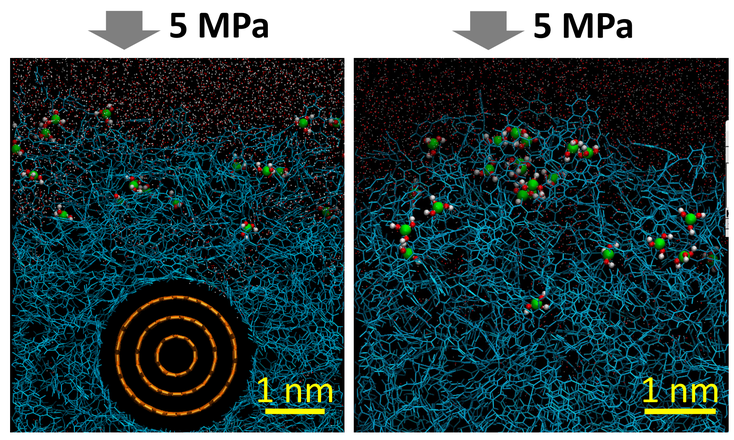


Water permeation is studied using a classical piston set-up

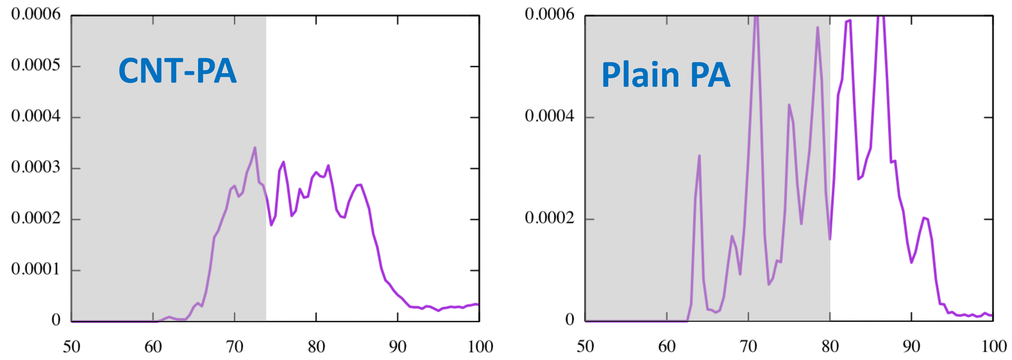




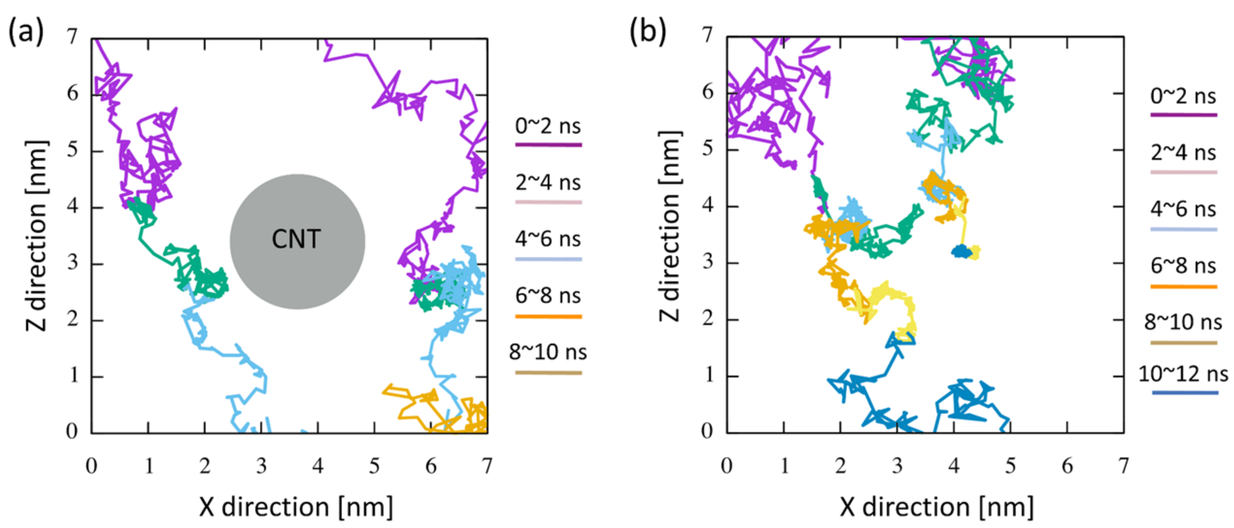
Boron permeation simulations



Boron density profiles in the membranes



Data is collected from classical atomistic molecular dynamics



Conclusions

CNT-PA membranes show a dense structure less prone to swell that can potentially have higher rejection rates of micropollutants

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-Water Diffusion Mechanism in Carbon Nanotube and Polyamide Nanocomposite Reverse Osmosis Membranes: A Possible Percolation-Hopping Mechanism, Takumi Araki, Rodolfo Cruz-Silva, Syogo Tejima, Josue Ortiz-Medina, Aaron Morelos-Gomez, Kenji Takeuchi, Takuya Hayashi, Mauricio Terrones, and Morinobu Endo, Phys. Rev. Applied 9, 024018 – Published 20 February 2018