Compaction of nitrogen-doped DLC membranes: elucidation of structural changes by molecular simulations

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Experimental evidence on the compaction of nitrogen-doped DLC based membranes, during their use in pressurized cross-flow systems for water desalination, demonstrated that their salt rejection performance could be improved from *ca*. 85% to *ca*. 96%, for a saline water with 3.2 wt.% NaCl concentration. The compaction occurs after a stabilization time during which the salt rejection performance reaches a maximum steady state, while observing a marginal decrease in water permeability capacity. Possible structural changes induced in N-DLC membranes are simulated by means of molecular dynamics, evaluating proposed configurations for original N-doped DLC cells. The results show that the compactability of DLC structure, along with its capability for rejecting solvated ions as well as allowing water molecules to pass through, are related with the nitrogen doping concentration, and with the sp^2/sp^3 hybridized bonds ratio within the amorphous carbon structure. The analysis shown here would contribute to the development of carbon-based membranes for water desalination and purification, as an alternative for conventional polymer-based membrane systems.