Abstract Submitted
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Nanoscale building blocks for the development of novel proton-exchange membranes fuel cells: A first-principles study[1] PHILIPPE F. WECK, EUNJA KIM, CHULSUNG BAE, NADUVALATH BALAKRISHNAN, University of Nevada Las Vegas — We propose a new type of sulfonated aromatic polyarylenes as candidate building blocks for proton-exchange membranes (PEMs) and investigate their electronic and structural properties using first-principles methods. Density functional theory calculations and ab initio molecular dynamics (MD) simulations suggest that desulfonation is limited at high temperatures, owing to the strong aryl-SO3H bond induced by the electron-deficient aromatic ring, and that the proposed polymers exhibit good thermomechanical stability due to the robust aromatic main-chain repeating unit. MD simulations of solvated sulfonated aromatic polyarylenes also emphasize the importance of the Grotthuss-type mechanism for the hydrated proton transport in the vicinity of the sulfonic acid groups. Simulations show that hydrated protons form fluxional defects in the hydrogen bonded network surrounding protogenic groups, the transport mechanism involving inter-conversion between the Eigen cation and the Zundel cation as limiting structures.

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