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Nuclear Quantum Effects in H^+ and OH^- Diffusion Along Confined Water Wires from Ab Initio Path Integral Molecular Dyanmics MARIANA ROSSI, Fritz Haber Institut der Max Planck Gesellschaft, MICHELE CERIOTTI, École Polytechnique Fédérale de Lausanne, DAVID MANOLOPOULOS, University of Oxford — Diffusion of H^+ and OH^- along water wires provides an efficient mechanism for charge transport that is exploited by biological systems and shows promise in technological applications. However, what is lacking for a better control and design of these systems is a thorough theoretical understanding of the diffusion process at the atomic scale. Here we consider H^+ and OH^- in finite water wires using density functional theory. We employ machine learning techniques to identify the charged species, thus obtaining an agnostic definition of the charge. We employ thermostated ring polymer molecular dynamics [1] and extract a "universal" diffusion coefficient from simulations with different wire sizes by considering Langevin dynamics on the potential of mean force of the charged species. In the classical case, diffusion coefficients depend significantly on the potential energy surface, in particular on how dispersion forces modulate O–O distances. NQEs, however, make the diffusion less sensitive to the underlying potential and geometry of the wire, presumably making them more robust to environment fluctuations [2]. [1] Rossi, Ceriotti, Manolopoulos, *JCP* **140**, 234116 (2014); [2] Rossi, Ceriotti, Manolopoulos, *JPCL* **7**, 3001 (2016).

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