AIMS Materials Science, 9(6): 919–938.
DOI: 10.3934/matersci.2022054
Received: 03 September 2022
Revised: 14 October 2022
Accepted: 25 October 2022
Published: 09 November 2022

http://www.aimspress.com/journal/Materials

Research article

Investigation of water desalination/purification with molecular dynamics and machine learning techniques

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Supplementary

In the following Figures, the mean square displacement (MSD) of the fluid solution is presented, for various cases of channel widths, electric field values, and wall wettability ratios. The values of the respective diffusion coefficient have been extracted from the MSD, according to Eq 7.

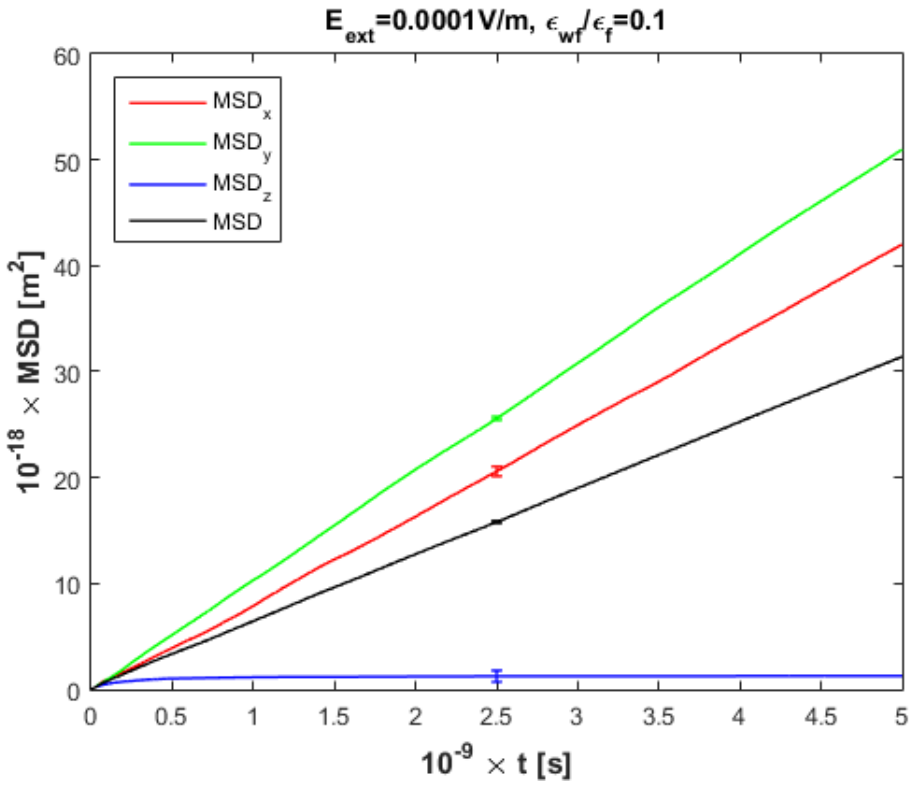

Figure S1. MSD for the h = 3 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 0.1$, and E_z = 0.0001 V/m.

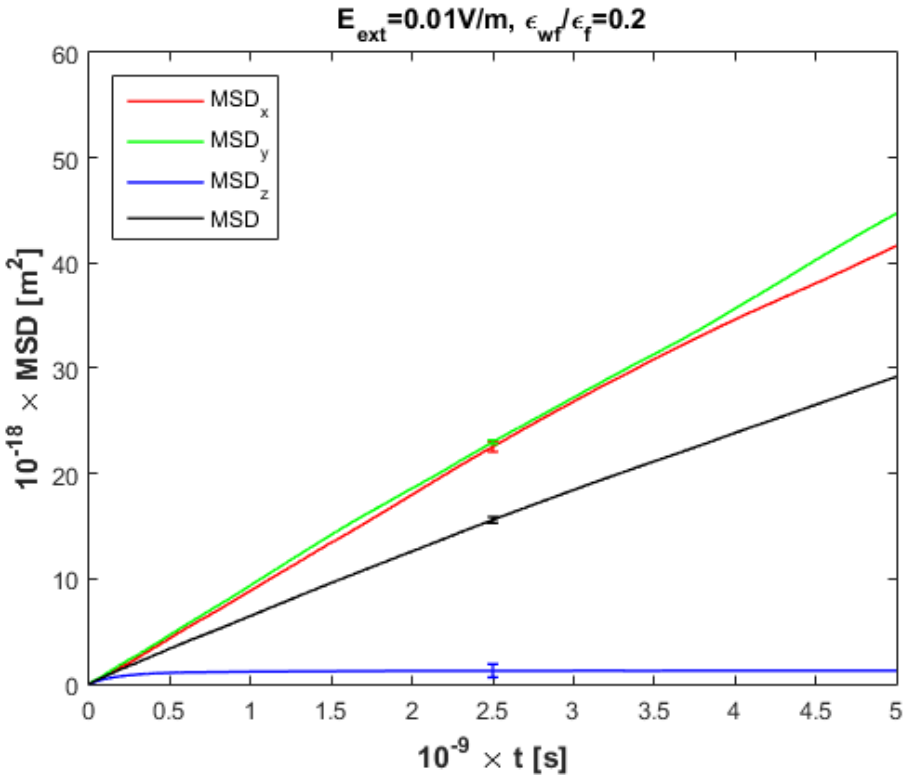

Figure S2. MSD for the h = 3 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 0.2$, and E_z = 0.01 V/m.

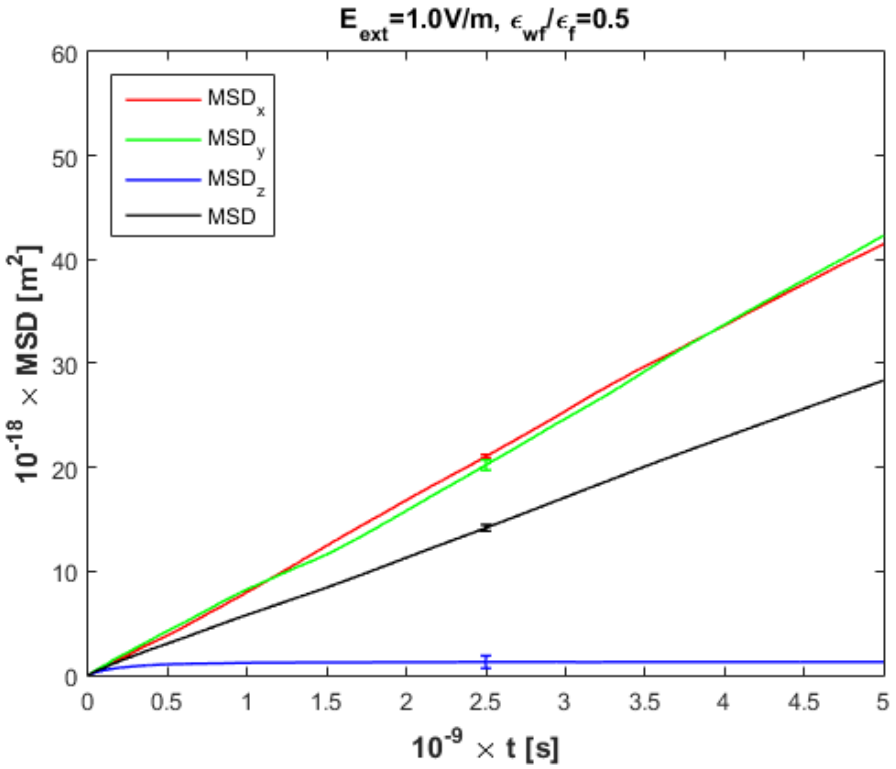

Figure S3. MSD for the h = 3 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 1.0$, and E_z = 0.5 V/m.

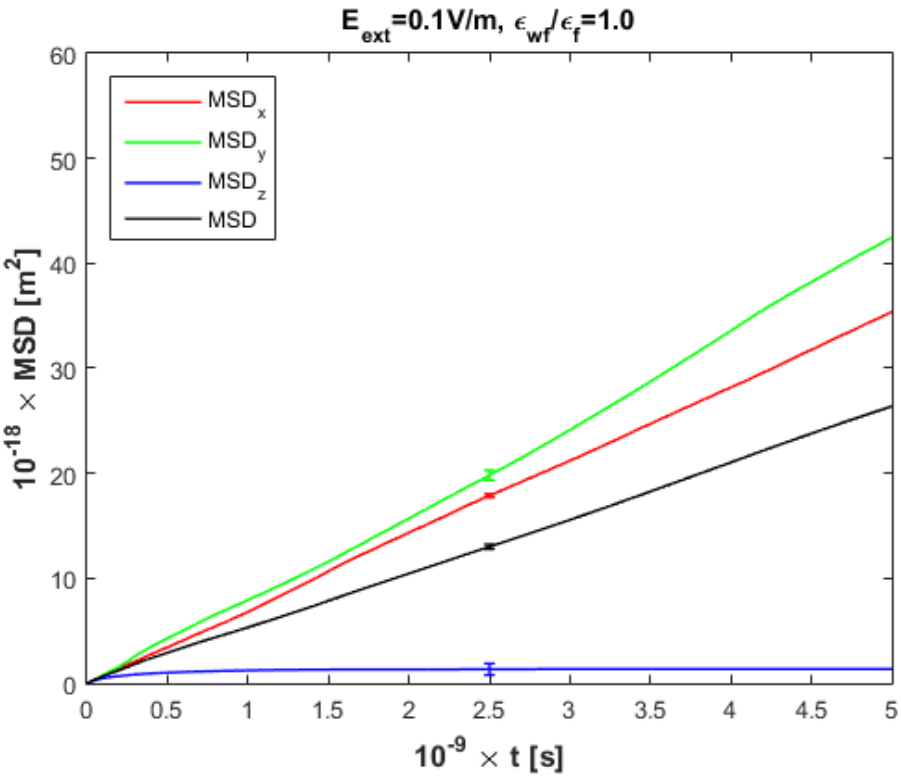

Figure S4. MSD for the h = 3 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 1.0$, and E_z = 0.1 V/m.

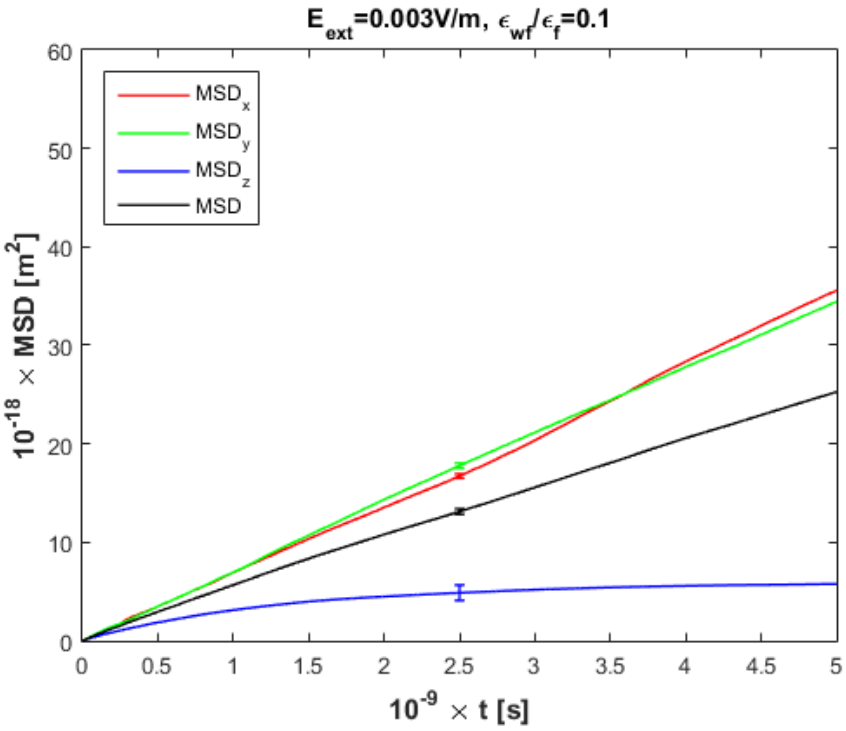

Figure S5. MSD for the h = 6 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 0.1$, and E_z = 0.0001 V/m.

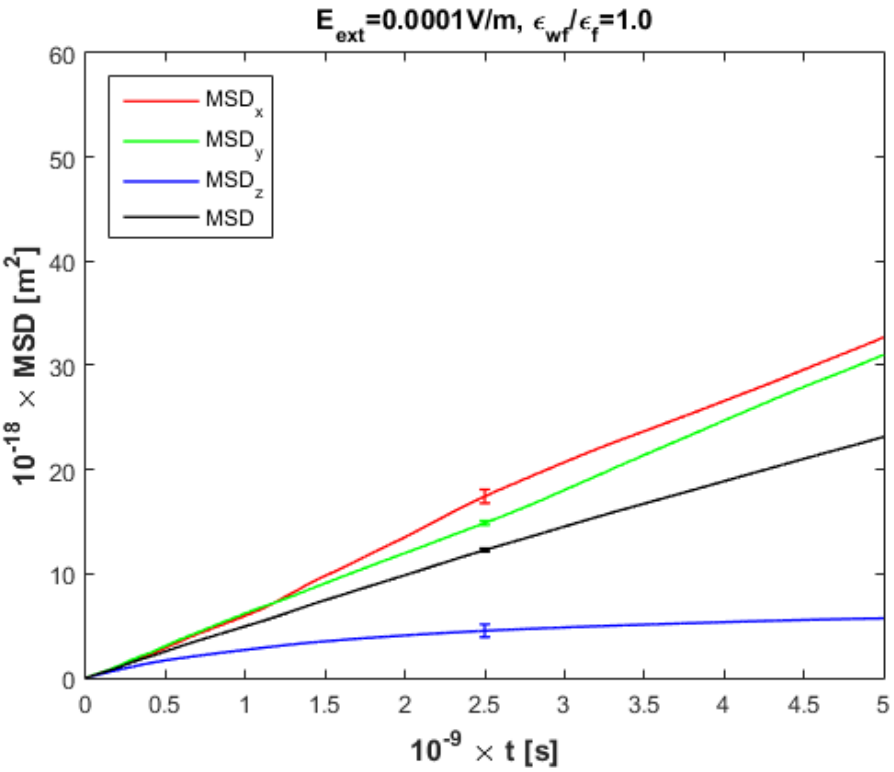

Figure S6. MSD for the h = 6 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 1.0$, and E_z = 0.0001 V/m.

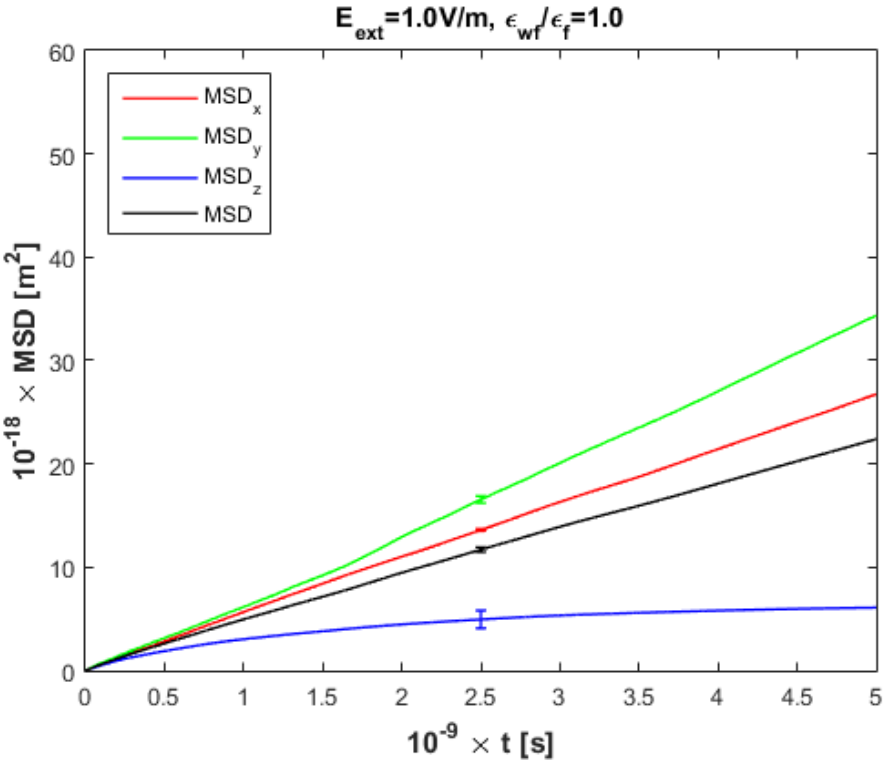

Figure S7. MSD for the h = 6 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 1.0$, and E_z = 1.0 V/m.

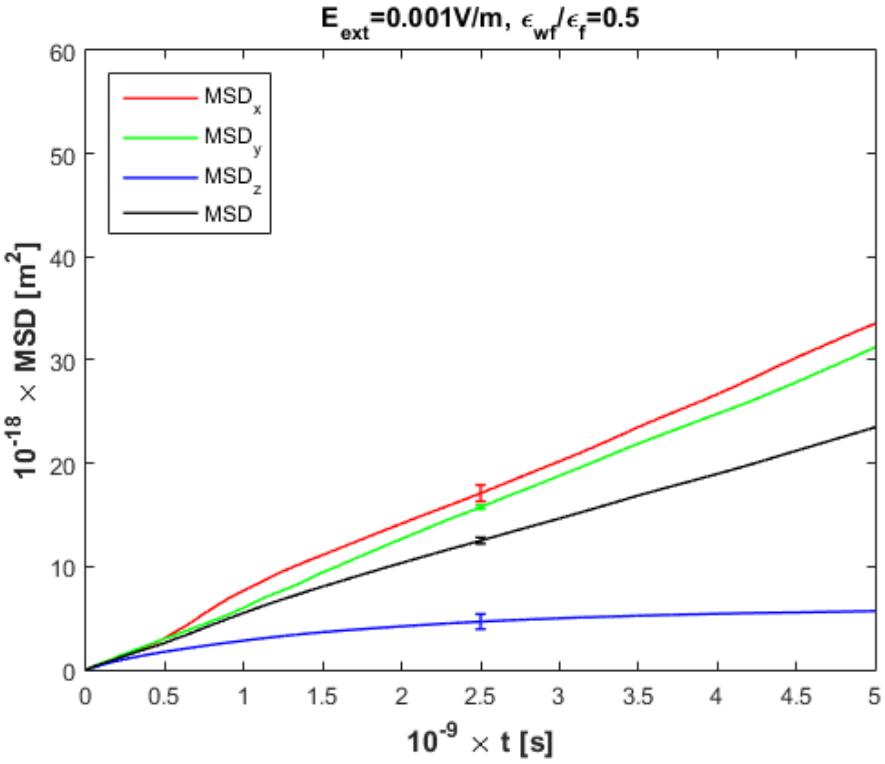

Figure S8. MSD for the h = 6 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 0.5$, and E_z = 0.001 V/m.

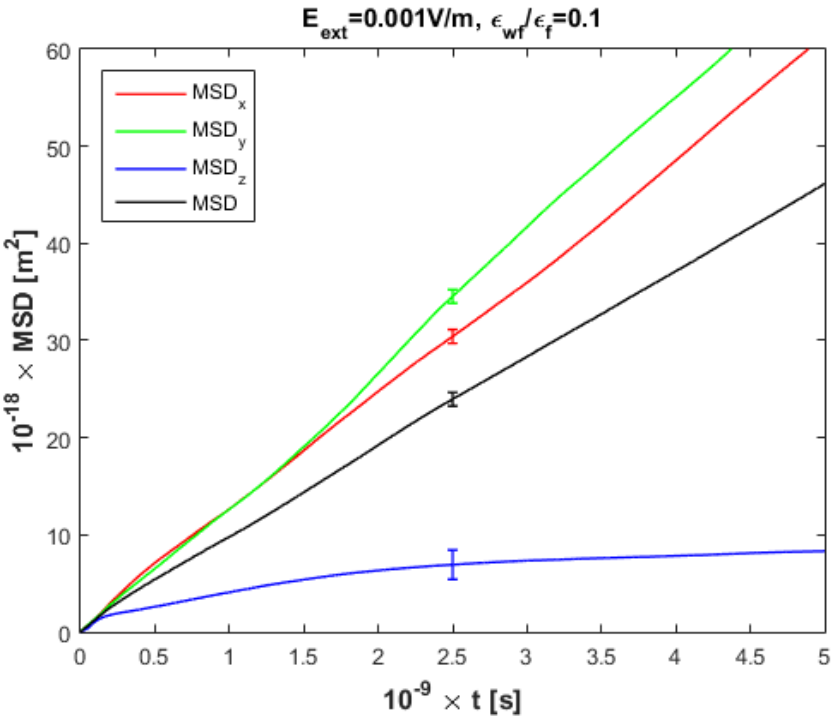

Figure S9. MSD for the h = 9 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 0.1$, and E_z = 0.001 V/m.

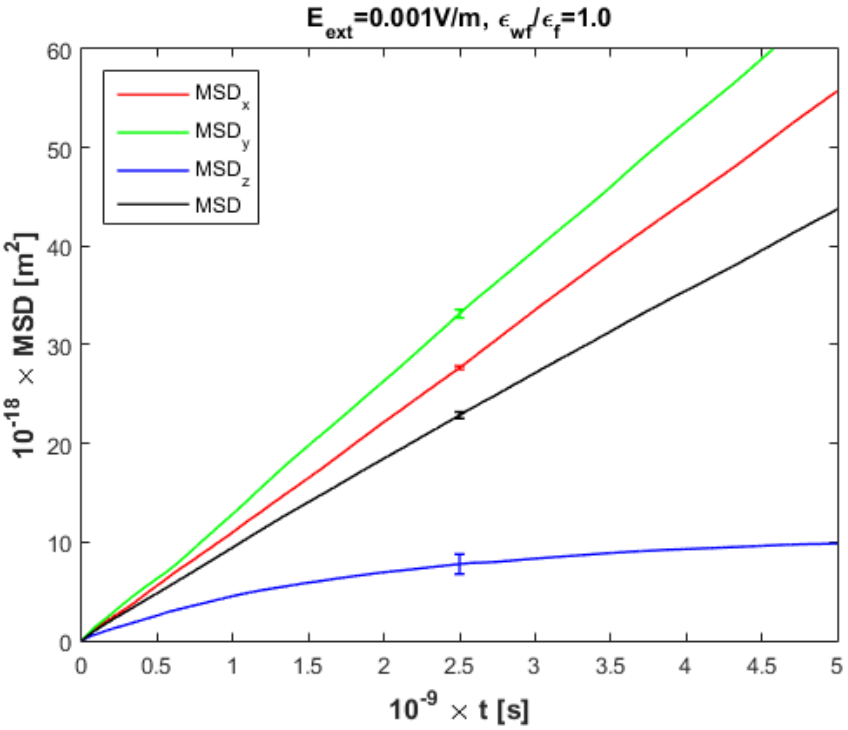

Figure S10. MSD for the h = 9 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 1.0$, and E_z = 0.001 V/m.

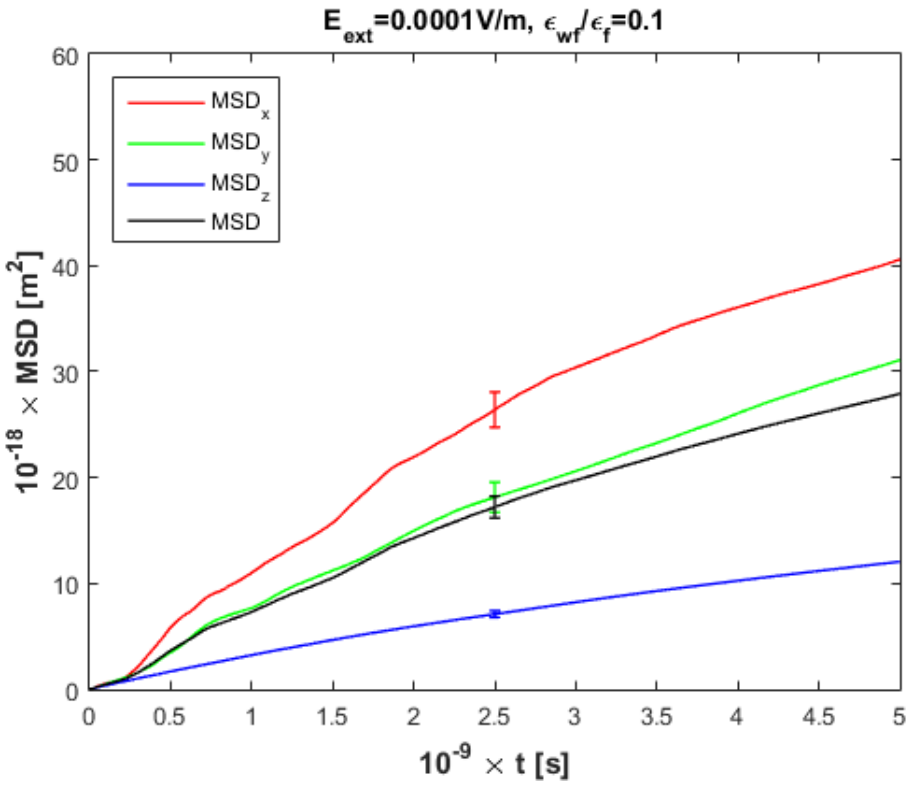

Figure S11. MSD for the h = 15 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 0.1$, and E_z = 0.0001 V/m.

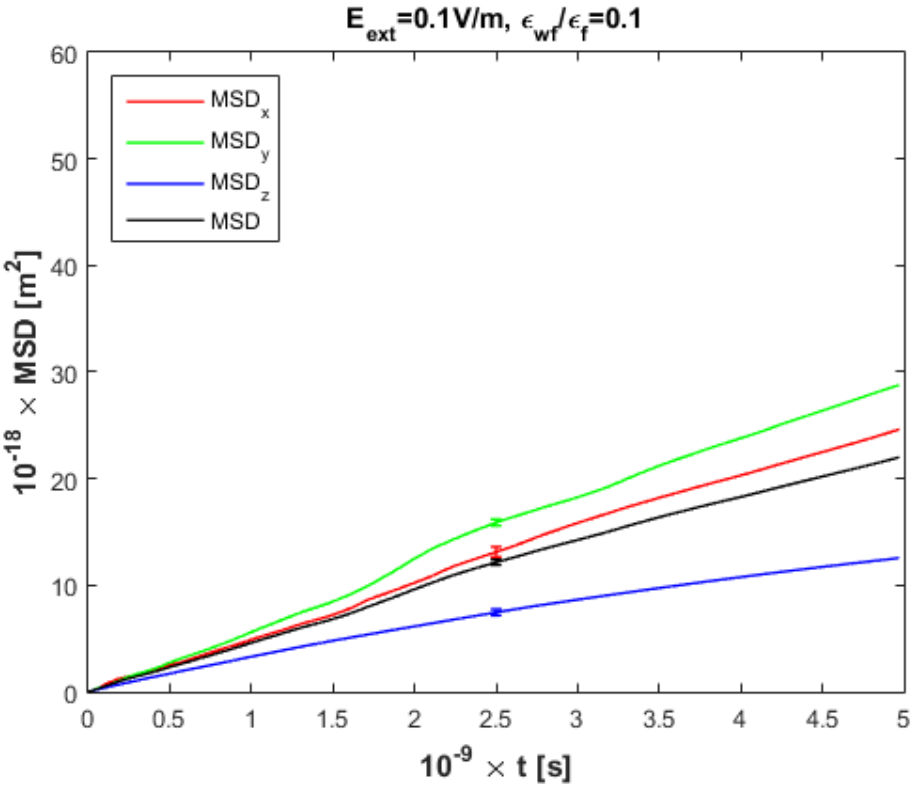

Figure S12. MSD for the h = 15 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 0.1$, and E_z = 0.1 V/m.

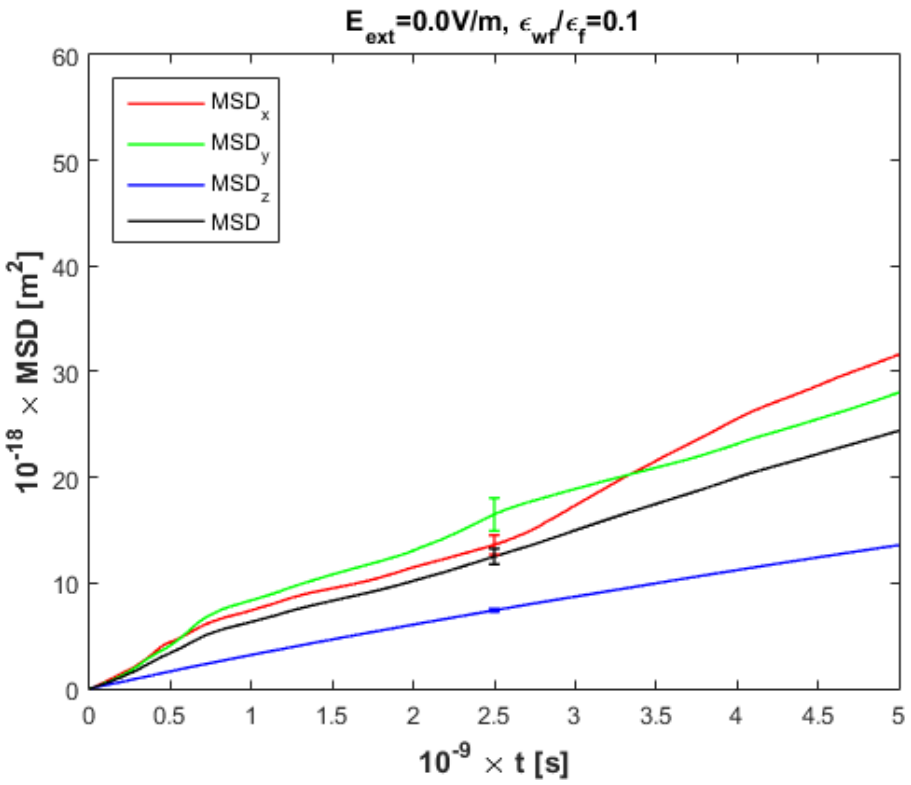

Figure S13. MSD for the h = 21 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 0.1$, and E_z = 0.0 V/m.

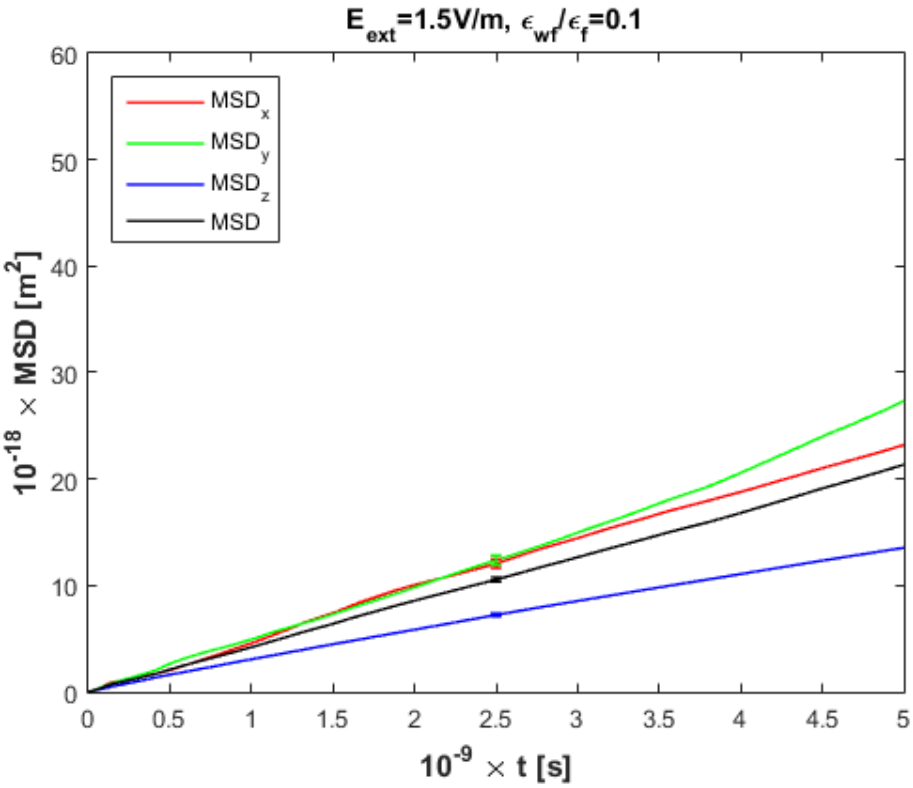

Figure S14. MSD for the h = 21 nm channel, with $\varepsilon_{wf}/\varepsilon_{ff} = 0.1$, and E_z = 1.5 V/m.