

# **The Role of Sulphonic and Phosphoric Pendant Groups on the Diffusion of Monovalent ions in Polyelectrolyte Membranes: A molecular dynamics study**

**Ismail Abdulazeez <sup>1,\*</sup>, Billel Salhi <sup>1</sup>, Nadeem Baig <sup>1</sup>, Isam H. Aljundi <sup>1,2,\*</sup> and Qing Peng <sup>3,4,5,\*</sup>**

<sup>1</sup> Interdisciplinary Research Center for Membranes and Water Security, King Fahd University of Petroleum and Minerals, Dhahran 31261 Saudi Arabia

<sup>2</sup> Chemical Engineering Department, King Fahd University of Petroleum and Minerals, Dhahran 31261 Saudi Arabia

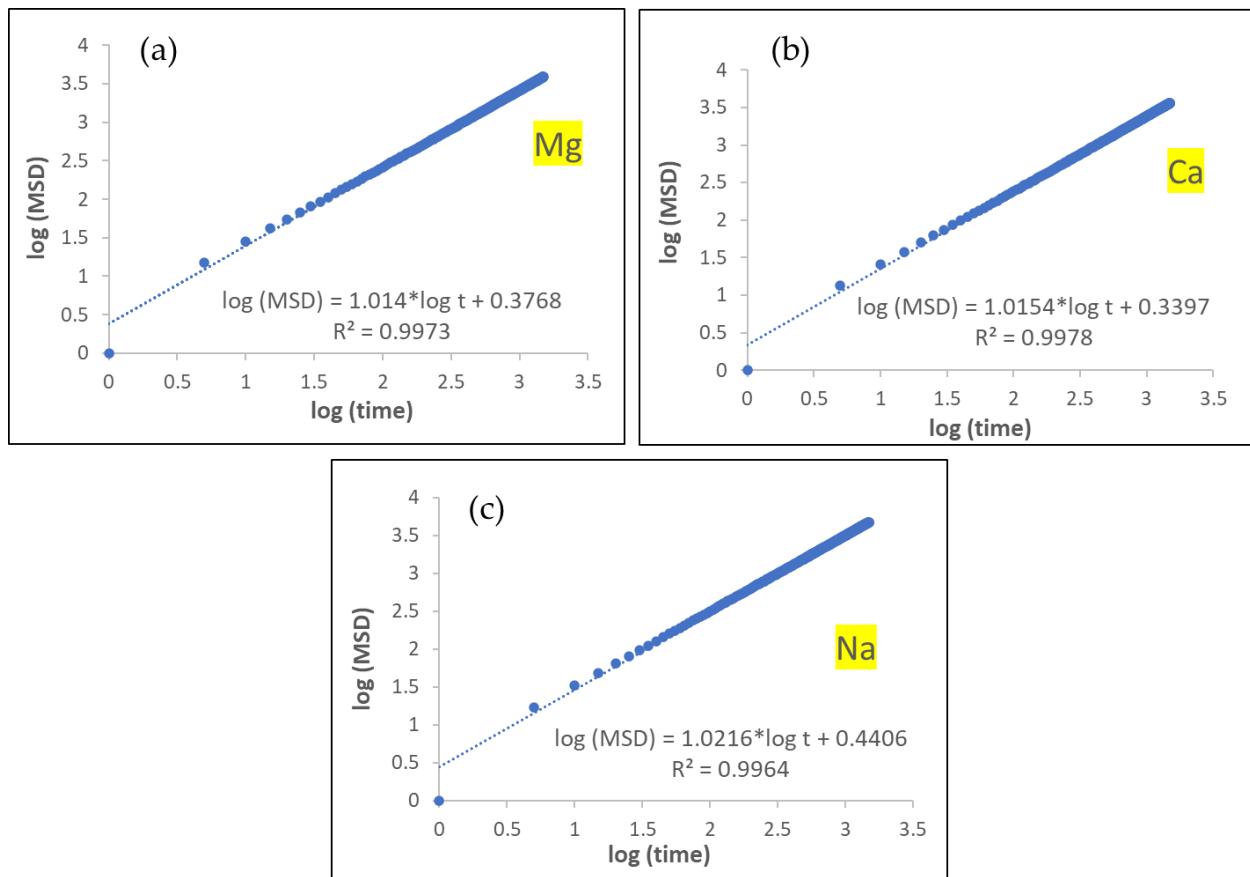
<sup>3</sup> Physics Department, King Fahd University of Petroleum and Minerals, Dhahran 31261 Saudi Arabia

<sup>4</sup> KACARE Energy Research and Innovation Center at Dhahran, Dhahran 31261 Saudi Arabia

<sup>5</sup> Hydrogen and Energy Storage Center, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

\* Correspondence: ismail.abdulazeez@kfupm.edu.sa (IA); aljundi@kfupm.edu.sa (I.H.A); qing.peng@kfupm.edu.sa (QP)

## **Supplementary Information**



**Figure S1.**  $\log(\text{MSD})$  vs  $\log t$  plots of (a)  $\text{Mg}^{2+}$ , (b)  $\text{Ca}^{2+}$  and (c)  $\text{Na}^{+}$  ions.