Supplementary information for:

Influences of electric fields on the operation of Aqy1 aquaporin channels: a molecular dynamics study

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The effects of water molecules models used in the simulation

1. **Application of the SPC/E water molecule model**

   The z- trajectory of water molecules in the channel for different cases, i.e. E=0, E=0.2 and -0.2 mV/nm, are shown in the panels of Fig. S1, when the water molecules interactions were computed with the aid of the extended single point charge (SPC/E) model. As can be seen, for the case of E=0, six water molecules entered the channel (from the downside) and by the end of the simulation, these water molecules remained in the channel without any net motion. For the case E=0.2 mV/nm, four water molecules entered the channel during the simulation, from which three molecules left the channel from the upside and one molecule from the downside of the channel. Subsequently, by exposing the channel to an electric field of amplitude -0.2 mV/nm, it was observed that during the simulation seven water molecules entered the channel, from which six molecules left the channel from the upside and one molecule from the downside of the channel.

   Figure S1

2. **Application of the TIP4P water molecule model**

   The above simulation performed again utilizing the transferable intermolecular potential 4 points (TIP4P) water model and the related results for the cases of E=0, E=0.2 and -0.2 mV/nm, are presented in the panels of Fig. S2. As can be seen, for the case of E=0, five water molecules from the downside entered the channel and stay in the channel up to the end of the simulation. For the case E=0.2 mV/nm, three water molecules entered the channel during the simulation, from which two ones left the channel from the upside and one molecule from the downside of the channel. Afterward, by applying E= -0.2 mV/nm on the channel, it was observed that during the simulation four water molecules entered the channel, and then left the channel from the upside of the channel.

   Figure S2

Figure S1 (SPC/E water model)

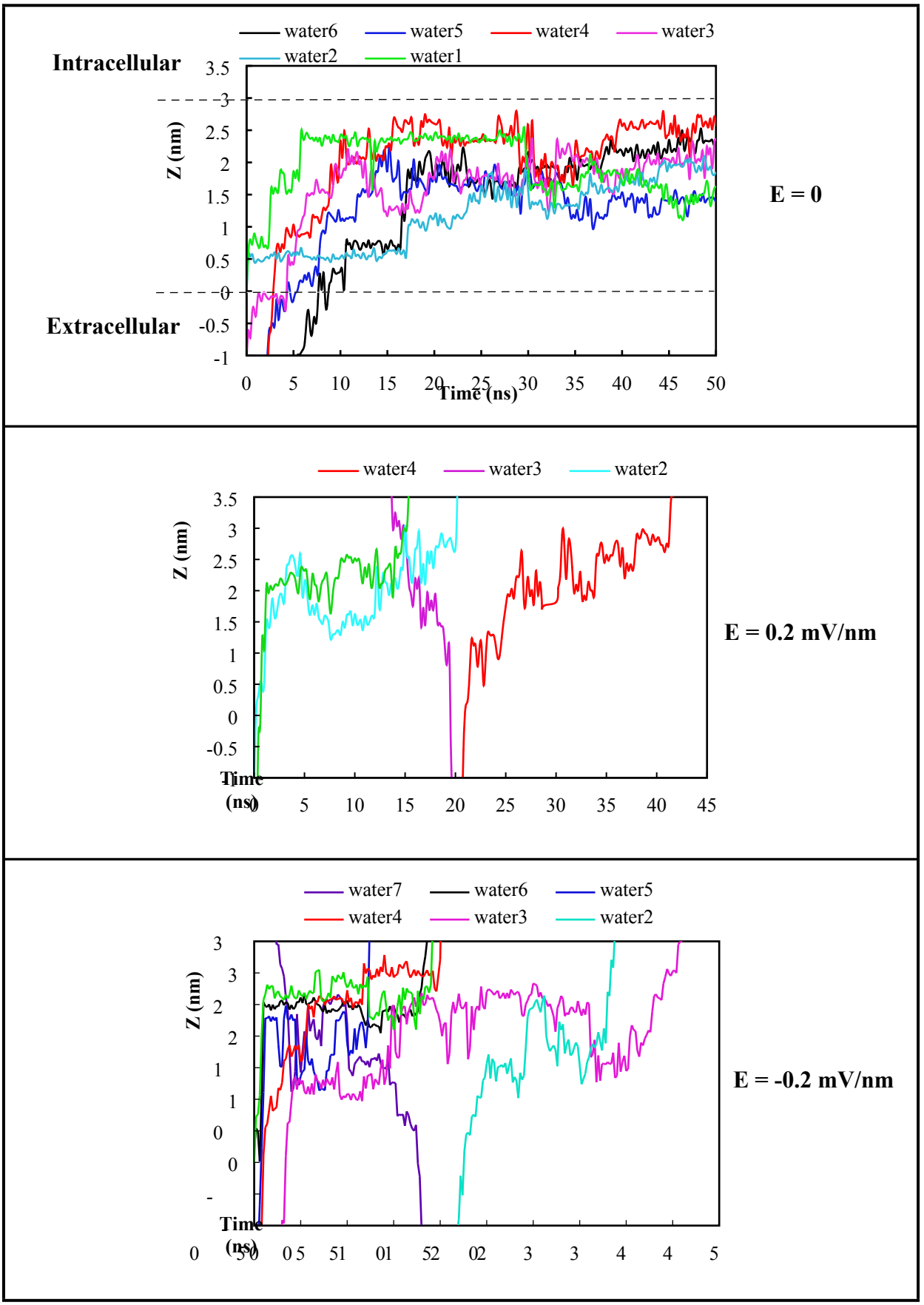
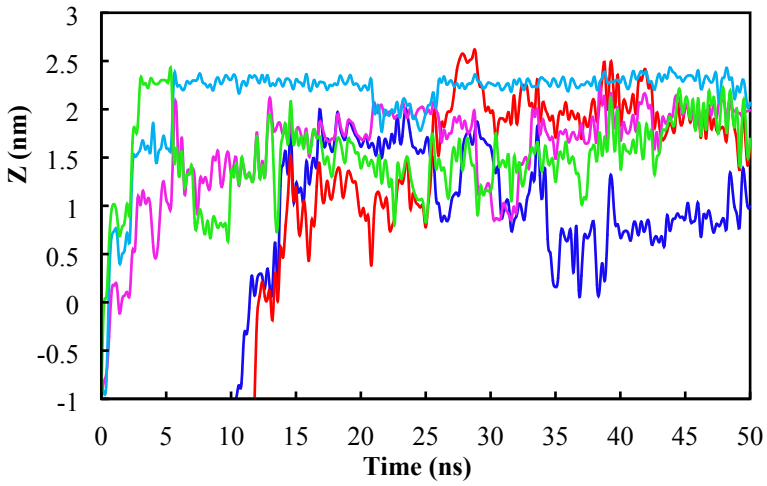
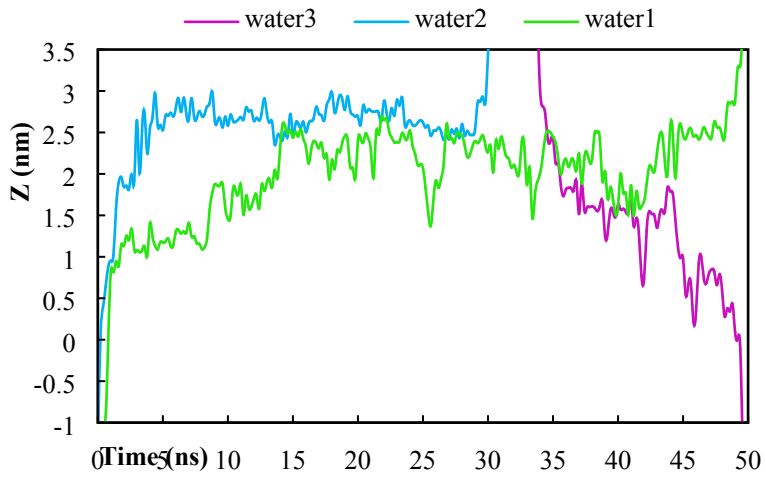


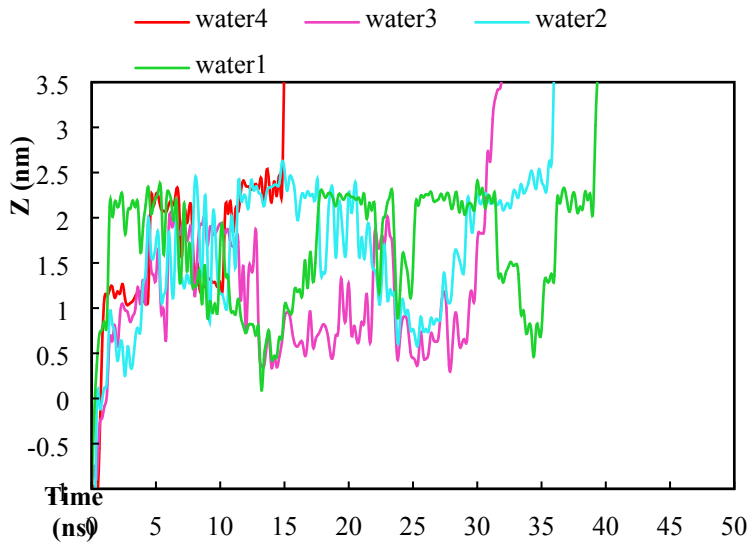
Figure S2 (TIP4P water model)



E=0



E=0.2 mV/nm



E=-0.2 mV/nm