Effect of a DC Electric field on the melting temperature, nucleation and ice growth rate of the TIP4P/ICE water model

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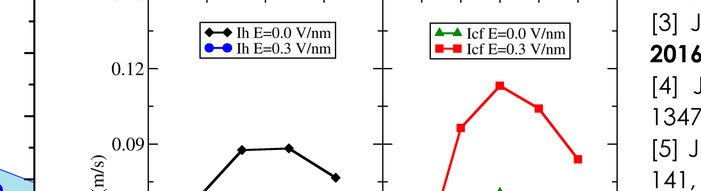
Introduction

Understanding the effect of electric fields on the thermal stability and phase transitions of water could have potential applications in the **food industry**, **cryopreservation**, and **environmental science**. In this work, we investigate the **effect of a static electric field** on the **melting temperature (T_m)**, **ice nucleation and ice growth rate** of two phases of ice, **hexagonal ice (Ih)** and **ferroelectric cubic ice (Icf)**, for the TIP4P/ICE water model. By means of **direct coexistence simulations**, we establish that **T_m of Ice Ih is shifted toward lower values**, whereas **T_m of Ice Icf grows**, becoming the most stable ice phase for sufficiently large values of the applied electric field. We also investigate ice nucleation for both ice phases under an external electric field and find that, **for a given supercooling** with respect to T_m, while **the field slows down the nucleation rate of ice Ih significantly, it barely affects that of ice Icf**, due to the enhanced ability of water molecules to orient favorably along the direction of the field in the latter phase. In terms of absolute temperature, overall ice formation is promoted by the electric field because it increases the melting point of ice Icf. Finally, we show how **the electric field slows down the crystal growth of Ice Ih and increases that of Ice Icf** by a factor of about two.

Methods

We simulate the **TIP4P/ICE**[1] water model using **GROMACS**, in the NpT ensemble, at $P = 1$ bar. We compute $\boldsymbol{T_m}$ by means of d**irect coexistence simulations.**

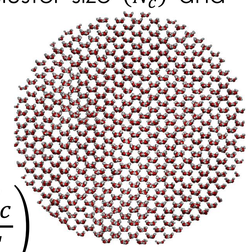


In order to calculate the **nucleation rate**, we employ the **seeding technique**[2,3] that combines **Classical Nucleation Theory** (CNT) and numerical calculations to establish the temperature at which a crystalline cluster is critical.

The CNT expressions for the critical cluster size (N_c) and the nucleation rate (J) are:

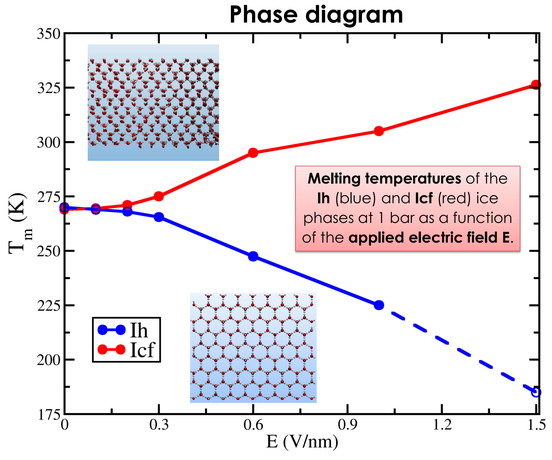
$$N_c = \frac{32\pi\gamma^3}{3\rho_s^2|\Delta\mu|^3}$$

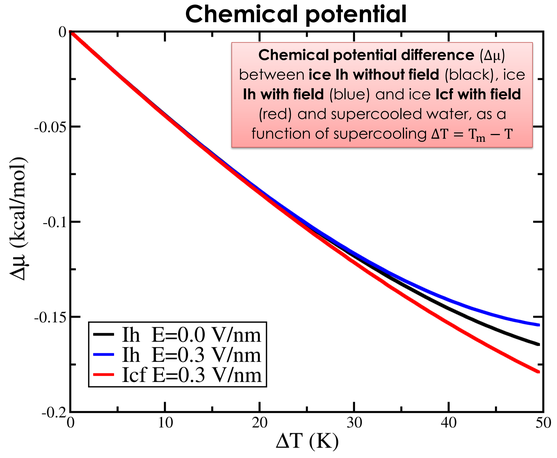
$$J = \sqrt{\frac{|\Delta\mu|}{6\pi k_B T N_c}} f^+ \rho_f \exp\left(\frac{-\Delta G_c}{k_B T}\right)$$

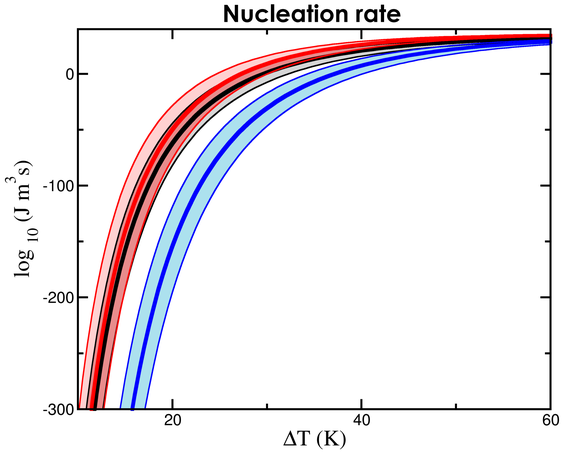


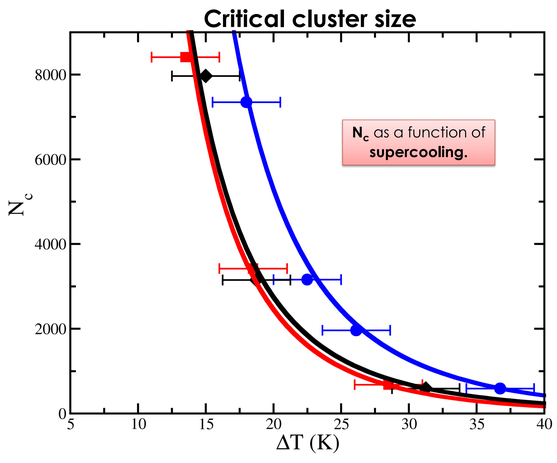
For the calculation of the ice-water interfacial free energy (γ) at coexistence, we use the **Mold Integration method**[4], by which we compute the reversible work $\Delta G = 2A\gamma$ needed to induce the formation of a crystal slab embedded in liquid water.

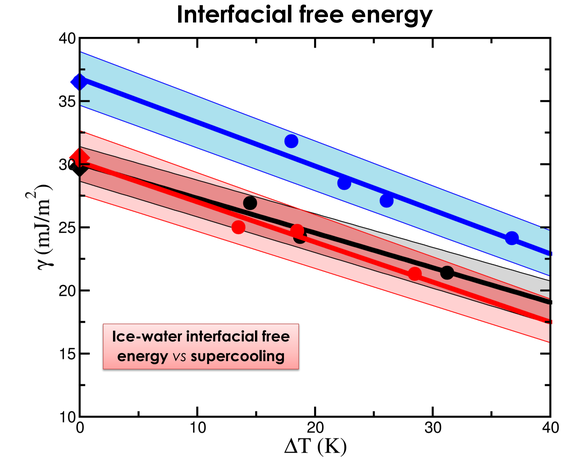
Results











Conclusions

- Ice **Ih** becomes **unstable** under a large electric field.
- A phase of **cubic ferroelectric ice** (**Icf**) becomes more thermodynamically stable, and has a much higher T_m.
- **For a given supercooling, the field slows down the nucleation rate of ice Ih significantly, but it barely affects that of ice Icf**.
- Water molecules can orient favorably with the field in ice Icf.
- In terms of absolute temperature, overall ice formation is promoted by the electric field.
- **The electric field slows down the crystal growth of Ice Ih and increases that of Ice Icf** by a factor of about two

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