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# Ultrahigh Oxygen Ion Mobility in Ferroelectric Hafnia

Ferroelectrics and ionic conductors are important functional materials, each supporting a plethora of applications in information and energy technology. The underlying physics governing their functional properties is ionic motion, and yet studies of ferroelectrics and ionic conductors are often considered separate fields. Based on first-principles calculations and deep-learning-assisted large-scale molecular dynamics simulations, we report ferroelectric-switching-promoted oxygen ion transport in HfO2, a wide-band-gap insulator with both ferroelectricity and ionic conductivity. Applying a unidirectional bias can activate multiple switching pathways in ferroelectric HfO2, leading to polar-antipolar phase cycling that appears to contradict classical electrodynamics. This apparent conflict is resolved by the geometric quantum-phase nature of electric polarization that carries no definite direction. This study highlights the geometric-quantum-phase attribute of spontaneous electric polarization in ferroelectric □□□21 HfO2 that displays dual-valued remnant polarization and single-valued piezoelectric response. Our molecular dynamics simulations demonstrate bias-driven successive ferroelectric transitions facilitate ultrahigh oxygen ion mobility at moderate temperatures, highlighting the potential of combining ferroelectricity and ionic conductivity for the development of advanced materials and technologies.

[1] Liyang Ma+, Jing Wu+, Tianyuan Zhu, Yiwei Huang, Qiyang Lu, and Shi Liu*, “Ultrahigh Oxygen Ion Mobility in Ferroelectric Hafnia”, Phys. Rev. Lett. 131, 256801 (2023)

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