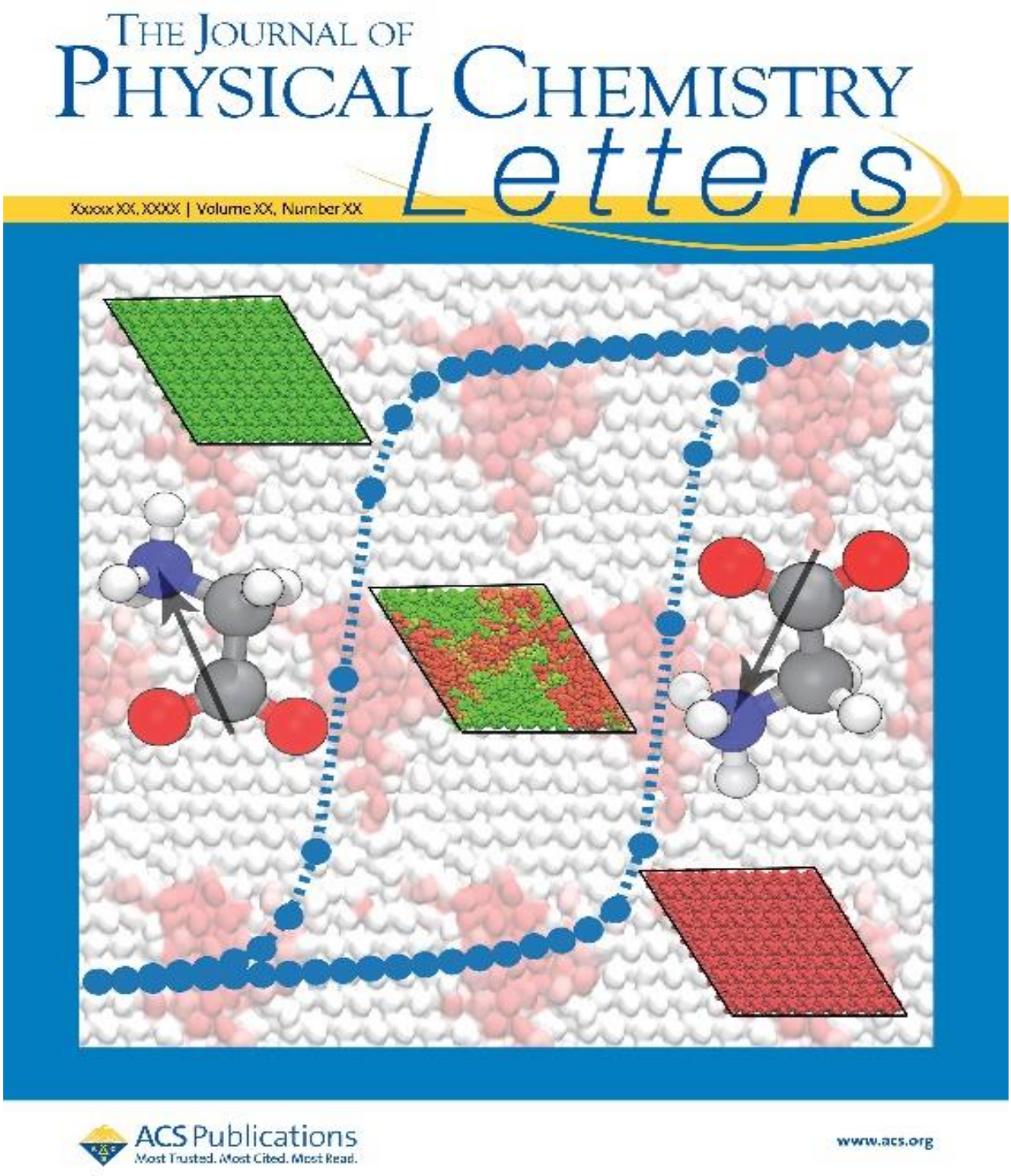


About the cover: **The dynamic process of the ferroelectric transition of γ-glycine**

The Journal of Physical Chemistry Letters has dedicated the cover of the Volume 10, Issue 6, March 21, 2019 to the study:

"**Bioferroelectric Properties of Glycine Crystals**"

https://pubs.acs.org.ccindex.cn/doi/10.1021/acs.jpclett.8b03837

Authors: A. Stroppa *et al.*

The article has also been selected for the special issue of Spotlights:

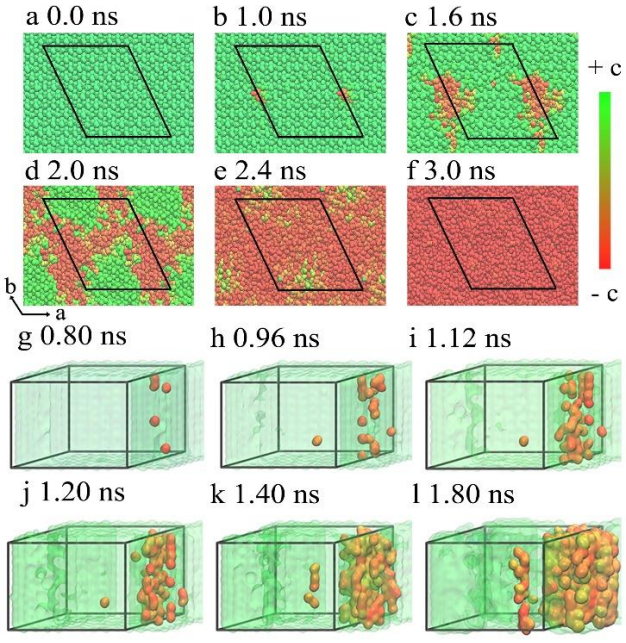
https://pubs.acs.org/toc/jpclcd/10/6

Biological ferroelectric materials are crossover stars in the fields of chemistry, biology, physics, and medicine, showing great potential in biosensing and disease diagnosis and treatment. Many biomaterials, including teeth and seashells, are known to have piezoelectric and ferroelectric properties, but the study of the general principles of ferroelectric switching has been limited by the complexity of biological materials.

Glycine, one of the simplest and smallest biological

molecules, presents nanoscale ferroelectricity and it can be synthetically modified to optimize properties. For these reasons, glycine is useful as a starting point in the design of functional materials.

The study is the result of the international collaboration of CNR-SPIN with Shanghai University and University of Pennsylvania. First-principles electronic structure calculations and molecular dynamics simulations were used to study the ferroelectric polarization of the β and γ phases of glycine. It is predicted that γ-glycine has a high spontaneous polarization, comparable to or even larger than that of traditional inorganic materials.



The study also reveals the microscopic dynamic mechanism of ferroelectric switching of γ-glycine through molecular dynamics simulations. A Curie temperature of 630 K is estimated with a required coercive field to switch the polarization states of 1 $V \cdot nm^{-1}$; these values are consistent with experimental evidence. This work

sheds light on the microscopic mechanism of electric dipole ordering in biomaterials, helping towards the materials design of novel bio-ferroelectrics.