Electronic Supplementary Information (ESI) for the manuscript "Experimental and theoretical Demonstration of Ferroelectric Anisotropy in a One-dimensional Copper(II)-based Coordination Polymer"

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Computational Methodology*:*

The partial geometry optimization of asymmetry unit of **1**, which was derived from X-ray single crystal diffraction, was performed by freezing non-hydrogen atoms at the level of B3LYP[1-3]/6-31G**.[4-6] The electric polarization of **1** at *c* axis shown in Table S1 was obtained from the generalized gradient approximations (BLYP,[1,7] BP86,[7,8] BPW91[7,9]), the hybrid functional methods (B3LYP,[1-3] B3P86,[3,8,10,11] B3PW91[3,10-12]), and the local spin density approach (SVWN5[13,14]) respectively. All calculation was performed with GAUSSIAN 03 package.[15]

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Table S1. The calculated electric polarization of **1** along *c* axis (|*PC|, $\mu C \cdot cm^{-2}$) obtained from diverse methods.

	B3LYP	BLYP	BP86	BPW91
6-31G**	1.262	1.138	1.151	1.149
	B3PW91	B3P86	SVWN5	
6-31G**	1.270	1.259	1.199	

[*] $\vec{P}_c = Z\vec{\mu}\cos(\vec{\mu} \wedge \vec{c})/V$ where *Z* is cell formula unit, $\vec{\mu}$ is the dipole moment in the asymmetry unit of **1**, $\vec{\mu} \wedge \vec{c}$ is the angle between $\vec{\mu}$ and $\vec{c}$, *V* is the cell volume of **1**。