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 BPW917,9), the hybrid functional methods (B3LYP,1-3 B3P86,3,8,10,11 B3PW913,10-12), and the local spin density approach (SVWN513,14) respectively. All calculation was performed with GAUSSIAN 03 package.15

References


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

<table>
<thead>
<tr>
<th></th>
<th>B3LYP</th>
<th>BLYP</th>
<th>BP86</th>
<th>BPW91</th>
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<tr>
<td>6-31G**</td>
<td>1.262</td>
<td>1.138</td>
<td>1.151</td>
<td>1.149</td>
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<td></td>
<td>B3PW91</td>
<td>B3P86</td>
<td>SVWN5</td>
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<td>6-31G**</td>
<td>1.270</td>
<td>1.259</td>
<td>1.199</td>
<td></td>
</tr>
</tbody>
</table>

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