Reply to Reviewer2

1、Usually, the results and methodology should not be mixed. They are typically described in separate parts by authors. The reviewed version of this paper does not change this. Section 2 still has a subsection describing the methodology of simulations and the results. These results should be explained in section for devoted to results.

A: We have adjusted the section.

2、The equation used to calculate the dielectric loss factor is not provided by the authors, and the uncertainty.

A: The dielectric loss in this paper is the tangent of the dielectric loss Angle, which refers to the energy consumed by the dielectric to convert electric energy into heat energy (in the form of heat) per unit volume within a unit time. The physical quantity characterizing the dielectric loss of dielectric material after the application of electric field is expressed by $\tan\delta$, δ is the dielectric loss Angle. The dielectric loss Angle is the Angle between the current vector and the voltage vector in the dielectric under the alternating electric field.

Uncertainty: The capacitance($\pm$0.1pF) and dielectric loss($\pm$5%$\pm$0.0001) were obtained directly during measurement

3、Authors do not describe what are the three types of polarization presented in the paper and why they present the three of them.

A：The final polarization results are shown in Table 1. Polarization result 1, Polarization result 2 and Polarization result 3 are three forms of polarization, and were given by the result document. The three columns of data in the table represent, from left to right, the polarizability results obtained when the molecule applies an electric field to the cubic angstroms, cubic centimeters, and atomic scales. The a.u. is a unit commonly used to add electric field in quantitative calculation, which can be converted with V/Angstrom. The conversion formula is as follows.

$$1\ \text{a.u.} = 51.423\ \text{V/Angstrom} \qquad (3)$$