Mechanism study of the conductivity characteristics of cellulose electrical insulation influenced by moisture

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Mechanism study of the conductivity characteristics of cellulose electrical insulation influenced by moisture

Haoxiang Zhao,1,a) Haibao Mu,1,b) Daning Zhang,1,c) Björn Baumeier,2,3,d) Huanmin Yao,1,e) Guangzhi Guo,1,f) and Guanjun Zhang1,g)

AFFILIATIONS
1 State Key Laboratory of Electrical Insulation and Power Equipment, School of Electrical Engineering, Xi’an Jiaotong University, Xi’an, China
2 Department of Mathematics and Computer Science, Eindhoven University of Technology, Eindhoven, The Netherlands
3 Institute for Complex Molecular Systems, Eindhoven University of Technology, Eindhoven, The Netherlands

a) xiang-yu@stu.xjtu.edu.cn
b) Author to whom correspondence should be addressed: haibaomu@mail.xjtu.edu.cn. Tel: +86 181 9225 1233
c) zdn_sdu@163.com
d) b.baumeier@tue.nl
e) yaohuanmin2010@163.com
f) ggzggz@stu.xjtu.edu.cn
g) gjzhang@mail.xjtu.edu.cn

ABSTRACT
Cellulose insulating paper is widely used in the power industry for its good electrical insulating properties. Moisture sharply increases its conductivity, which directly leads to the weakening of insulation performance and greatly increases the risk of subsequent electric field distortion and insulation breakdown. This paper focuses on the microscopic mechanism of moisture changing the characteristics of charge transport in cellulose insulation and attempts to reveal the related conductivity mechanism. To achieve this purpose, microscopic and macroscopic perspectives are integrated and several simulation and experimental methods are utilized comprehensively. The molecular dynamics simulation results showed that most water molecules in damped cellulose were individually and uniformly adsorbed on the hydroxyl groups by hydrogen bond, and the quantum chemistry computation results showed that the lowest unoccupied molecular orbital more appeared on the water molecule and the corresponding density of state increased. Then, experimentally, it was confirmed that the trap energy level decreased by the thermally stimulated current method. On this basis, the promotion effect of moisture on charge transport is predicted and verified by polarization and depolarization current methods. As the moisture content increased, more charge carriers escaped from the trap by hopping and participated in long-range continuous charge motion. Therefore, after dampness, the current of cellulose insulating paper increased exponentially with the increase in electric field strength, which was consistent with the hopping conductivity mechanism.

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I. INTRODUCTION
Cellulose paper is an important electrical insulating material and has been widely used in oil-filled electrical power equipment,1 playing a vital role in ensuring the electricity supply of our society. Nevertheless, good insulation performance presupposes that the cellulose is in an extremely dry state,2 while cellulose paper is hydrophilic and easy to get damped by moisture ingressed from the external environment and generated during the aging process,3,4 and a small amount of moisture irreversibly and severely deteriorates the insulation properties of the power equipment.5,6 As one of the most important deterioration characteristics, conductivity...
increases rapidly with a small amount of moisture in cellulose paper. However, the microscopic mechanism where moisture increases the conductivity of cellulose paper is still unclear. This mechanism issue not only directly leads to a lack of theoretical support for the accurate evaluation of insulation deterioration but also hinders further mechanistic exploration of electric field distortion and insulation prebreakdown. More importantly, the uncertainty of this mechanism has resulted in a lack of theoretical guidance for cellulose polymer modification that is dedicated to improve the electrical insulation performance.\(^{11,12}\)

The exploration of the conductivity mechanism started with the experimental law. Sha Yanchao et al. \(^{13}\) and Chi Minghe et al. \(^{14}\) studied the influence of the electric field and moisture on the conductivity of cellulose paper, respectively, but they did not explain the more in-depth charge transport and the mechanism. Hao Jian et al. \(^{15}\) found that the accumulation and dissipation of space charge in the cellulose paper were accelerated with increasing moisture content, which was consistent with the promotion of the conductance process. In the oil-filled cellulose paper insulating power equipment, more than 99% of the moisture is in the paper rather than the oil,\(^{16,17}\) and a plausible explanation is that the liquid water dissolves impurity ions and promotes the conductance process by increasing the carrier concentration.\(^{18}\) However, this plausible explanation is still questionable. When the moisture content of the cellulose paper reaches 6% in the operating power equipment, its insulation performance has severely deteriorated and the equipment should be taken out of service.\(^{19}\) Thus, the actual moisture content in the cellulose insulating paper is below 6%, and it is a very low moisture content to dissolve impurity ions.

The microscopic moisture adsorption characteristics in cellulose play an important role in addressing the issue of charge transport and the conductivity mechanism influenced by moisture. Using terahertz dielectric spectroscopy, hydrogen bonding has been found to play a crucial role between cellulose and moisture.\(^{20}\) Utilizing broadband spectroscopy, different types of hydrogen bonds are found in damped cellulose insulation.\(^{21}\) However, by these experimental methods, different types of hydrogen bonds cannot be identified and analyzed in detail. Moreover, the effect of hydrogen bonding on charge transport and the conductivity mechanism cannot be further explored microscopically.

Instead, a combination of molecular dynamics (MD) simulations with quantum chemistry (QC) calculations can provide such microscopic insight.\(^{22-24}\) MD allows a detailed study of hydrogen bond characteristics at the molecular scale,\(^{25}\) so it is a powerful tool for exploring microscopic moisture adsorption characteristics. Due to the disordered nature, the charge transport in cellulose is likely of the hopping type between trap localized states.\(^{26,27}\) Therefore, the conductance process is influenced by trap energy levels, which can be obtained from QC. Jiang Zhihui et al.\(^{28}\) analyzed the increase in the trap energy level based on the density of state (DOS) obtained from the QC. For damped cellulose paper, the adsorbed moisture may influence the trap energy level; thus, the combination of MD and QC can offer some important insights into the revelation of the conductivity mechanism.

Traps link the microscopic and the macroscopic. After microscopic computational studies, electrical experiments provide further macroscopic exploration. Based on the dielectric response theory and appropriate processing of experimental results,\(^{27-29}\) the actual change of trap energy level of cellulose paper influenced by moisture can be obtained by the thermally stimulated current (TSC).\(^{30}\) and the detailed characteristics of charge transport can be extracted from the polarization and depolarization current (PDC).

Aiming to reveal the mechanism where the conductivity properties of cellulose paper were influenced by moisture, micro- and macro-points of view were integrated and several simulation and experimental methods were utilized in this study. First, the microscopic moisture adsorption characteristics in cellulose were obtained by MD. Then, the possible changing trend of the corresponding trap localized states is analyzed by QC. Furthermore, by electrical experiments, the actual change of the trap energy level of the cellulose paper influenced by moisture was obtained, and the effects of moisture on charge transport were predicted and verified well. Finally, based on the hopping conductance model, the conductivity characteristics of cellulose insulation influenced by moisture were explained deeply.

### II. MATERIAL AND METHODS

#### A. Computational details

Cellulosic materials are typically composed of intermittent crystalline and amorphous cellulose regions,\(^{31,32}\) and the proportion of amorphous regions in the insulating paper is considerably 30%–50%.\(^{33,34}\) Moisture content of the cellulose insulating paper in the actual operating power equipment is very low, which corresponds to the initial stage of moisture adsorption in cellulose and occurs mainly in the amorphous region.\(^{35,36}\) In addition, for polymer dielectrics, the trap localized states are mainly distributed in the amorphous region.\(^{37-39}\) Therefore, microscopic moisture adsorption in the amorphous region and its effect on trap localized states were explored by MD simulations and QC calculations, respectively.

The MD simulations were performed by Gromacs\(^{40}\) using the Gromos 54a7 force field.\(^{41}\) Previous studies have shown that the MD results are independent of both the initial chain length and initial density of the initial length.\(^{42,43}\) Thus, in this work, each cellulose chain consisted of 10 cellobiose repeats, and five cellulose chains were packed into a cubic box, which was set with periodic boundary conditions.\(^{44}\) Regarding the actual damp condition of the cellulose paper insulating power equipment,\(^{45}\) the moisture content was set to 0%, 1%, 2%, 3%, 4%, 5%, and 6% by randomly adding the SPC/E described water molecules to the cubic box. The models were set with periodic boundary conditions at x, y, and z directions. The long-range coulomb interactions are calculated by particle mesh Ewald (PME) with a cut-off of 1 nm and with Fourier spacing of 0.12 nm. The integrator is a leap frog. The dynamic relaxation was performed at constant temperature/pressure (298.15 K/1.013 25 bar) with a velocity-rescale thermostat (time constant 0.2 ps) and a Berendsen barostat (time constant 0.5 ps). The total relaxation time is 1 ns and the time step is 0.002 ps.

The QC calculations were performed by the ORCA quantum chemical package\(^{46}\) based on the density function theory (DFT). The B3LYP\(^{47}\)/def2-SVP\(^{48}\) level was employed in all single-point energy and geometry optimization calculations. The objects of QC calculations were two local molecular systems centered on the moisture adsorption site and were intercepted from the MD relaxed...
amorphous cellulose. The Multiwfn and VMD software were used to visualize the calculation results of the molecular orbital isosurfaces.46,47

B. Experimental section

Referring to the standard IEC60422, the cellulose paper was dried in an oven at 90 °C/50 Pa for 48 h and then impregnated in the dry insulating mineral oil. The moisture content of the oil-immersed paper samples was controlled at gradient content by the weighing method.5 The final moisture content of samples was tested by the Karl Fischer coulometer KFT831 according to the standard IEC60814. The gradient moisture contents were 0.74%, 1.82%, 2.97%, and 4.63%, respectively.

The principle of TSC is based on the energy-dependent characteristics of the charge de-trap process. The standard TSC curves were measured by the Concept 90.30 The injected charges were first cryogenically frozen in the trap and then excited by an increasing temperature. During the heating process, the charges in the traps of different energy levels escape sequentially, forming several current peaks. The current peak is expressed as Eq. (1), based on which the trap parameters of the dielectric can be extracted.48

\[
I(T) = A \exp \left[ -\frac{H}{kT} - \frac{B}{\beta} \int_{T_0}^{T} \exp \left( -\frac{H}{kT} \right) dT \right], \tag{1}
\]

where \(A\) and \(B\) are constants, \(k\) is the Boltzmann constant, \(T\) is temperature, \(T_0\) is the initial temperature, \(\beta\) is the heating rate, and \(H\) is the trap energy level.

PDC was measured by Keithley 6517A. During the measurements, the samples were placed in an oven, where the temperature inside is stabilized at 30 °C. The polarization current \(i_p\) was the total current flowing through the sample under a DC voltage. The depolarization current \(i_d\) was the total current released in the opposite direction after the voltage was removed. According to the standards IEC61620 and IEC60247, all current results within 1000 s were used to characterize the transient conductance process, and the steady current value at the 1000th second was used to calculate the conductivity. The compositions of \(i_p\) and \(i_d\) are shown in Eqs. (2) and (3), respectively, where \(i_a\) is the absorption current, \(i_\sigma\) is the steady conductance current, and \(i_a'\) is the desorption current.49

\[
i_p = i_a + i_\sigma, \tag{2}
\]
\[
i_d = i_a'. \tag{3}
\]

III. RESULTS AND DISCUSSION

A. Role of moisture in changing the trap energy level of cellulose

1. The moisture adsorption characteristics in cellulose

The final molecular configuration of dry amorphous cellulose is shown in Fig. 1(a), and the side of the final cube is 2.69 nm. The density reached the final converged value after 200 ps as shown in Fig. 1(b). The average density of the final construction was 1.38 g cm\(^{-3}\), which was comparable to the reported computational

![FIG. 1. Molecular configurations of dry amorphous cellulose (a), density of dry amorphous cellulose as a function of time (b), radial pair distribution function g(r) of heavy atoms (C and O atoms) in the dry amorphous cellulose model (c), amorphous cellulose with 6% moisture content (d), and the hydrogen bonds in amorphous cellulose with 6% moisture content (e).](image-url)
The result of 1.39 g cm$^{-3}$ and the experimental result of 1.48 g cm$^{-3}$. The experimental object naturally contains some crystalline regions; so the experimental result is a little bigger than that of the calculated result. The radial pair distribution function $g(r)$ of heavy atoms (C and O atoms) is shown in Fig. 1(c). All the important peaks appeared at short distances and no peak appeared at distance larger than 5 Å, which was consistent with the amorphous structure principle of long-range disorder and short-range order. This result indicated that a reasonable amorphous cellulose system had been established. Due to the limitation of paper length and similarity of results, only the MD results of cellulose with a moisture content of 6% are shown in Figs. 1(d) and 1(e). For easy identification, the water molecules were represented as spherical and the cellulose as rod-shaped. The O, H, and C atoms were cyan, red, and white, respectively. From Fig. 1(d), the water molecules are uniformly distributed and almost no water clusters are formed. In Fig. 1(e), the red dashed marked hydrogen bonds are judged by a cut-off angle of 30° and a distance of 0.35 nm. Also, the hydrogen bonds were uniformly and individually distributed, which indicated that almost no water clusters were formed even in the worst dampness case.

Hydrogen bonding plays a critical role in the detailed analysis of moisture adsorption characteristics. There were three kinds of hydrogen bonds in damped cellulose: the hydrogen bond between water molecules (HB-WW), between cellulose and water molecules (HB-CW), and between cellulose molecules (HB-CC). All types of hydrogen bonds are shown in Fig. 2(a), and it can be seen that the hydrogen bonds associated with cellulose are formed by hydroxyl groups. In Fig. 2(b), the numbers of different hydrogen bonds that changed along the increasing moisture content are counted. When the moisture content increased from 0% to 6%, the average number of HB-WW hardly increased, while the average number of HB-CW increased significantly. The increases of HB-CW and HB-Total were consistent, indicating HB-CW contributed most of the hydrogen bond increase. The hydrogen bonding statistics showed that most of the water molecules were individually adsorbed on the hydroxyl groups of cellulose rather than forming water clusters. When the moisture content was beyond 3%, the HB-CC began to decrease while the HB-WW began to increase. This consistency suggests that the water clusters began to form, which may lead to a decrease in the mechanical properties of the insulating paper, although the HB-CW is still dominant in the water-related hydrogen bonds. From Fig. 2(b), the cellulose-related hydrogen bonds HB-CC + CW increased at a slower rate when the moisture content increased. When the moisture content increased from 5% to 6%, there was little increase in the HB-CC + CW, which indicated that the cellulose-related hydrogen bonds appeared to tend to saturate. The saturation tendency of cellulose-related hydrogen bonds may be because the limited available exposed hydroxyl sites had been almost occupied during the moisture increase.

In summary, most water molecules in damped cellulose insulation were individually adsorbed to the hydroxyl groups, and the liquid water began to form when the cellulose insulating paper was severely damped. This moisture adsorption characteristic matched the formation analysis of liquid water (water clusters) based on the hydrogen bond energy and the liquid water cohesive energy in the research by Chen et al. Also, these results can well explain the diffuse-reflectance spectroscopic characteristics in the previous study: When the moisture content was low, the water molecules were uniformly distributed and almost no water clusters were formed so that the characteristic peak of liquid water in the spectrum of damped insulating paper was extremely small when the moisture content was below 7%. Based on this moisture adsorption characteristic, the conductance process could not be facilitated by dissolving impurity ions and water dissociating. The deteriorating effect of small amounts of moisture on conductivity needs to be considered from factors other than dissolved ions in liquid water.
2. The effects of moisture on the change of trap localized states

In a broad sense, the trap in the dielectric is a localized state close to the energy gap and it has a critical impact on the charge transport process. For polymer dielectrics and physical or chemical structural defects, various polar and ionic groups belong to the category of traps. As an electronegative group, the hydroxyl group has been confirmed to be with the nature of the trap. The water molecules adsorbed on hydroxyl groups would inevitably affect the corresponding trap localized states.

From the dry and damped MD relaxed cellulose, we extracted two local molecular systems centered on the moisture adsorption site for QC calculations, as shown in Figs. 3(a) and 3(c). The colored cellulose fragments at the center of the two systems were the same one, which were the focus of our investigation. The outer layer molecules of the central cellulose fragment were also retained and marked in gray. During the next structure optimization computation, non-hydrogen atoms in these outer molecules were frozen to maintain the molecular environment of the central cellulose fragment. The difference between these two systems was whether the water molecule was adsorbed on the hydroxyl group.

![Diagram showing extracted local molecular systems and DOS for QC calculations](image-url)
The density of state (DOS) of these two central cellulose fragments and the isosurface of the lowest unoccupied molecular orbital (LUMO) are shown in Figs. 3(b) and 3(d). The LUMOs were framed in blue, and the according peaks were marked with black dashed lines. The values of the energy level were also indicated in the figure. The LUMO was most likely to become an electron trap by gaining electrons, and from Fig. 3(b), it is mainly distributed in the hydroxyl group. After water adsorption shown in Fig. 3(d), as predicted, part of the LUMO appeared on the water molecule. This change characteristic was also consistent with the DOS results. Comparing Figs. 3(b) and 3(d), the DOS of LUMO is enhanced by the adsorbed water molecule, whose DOS is marked in green. The energy level of LUMO decreased by 0.15 eV from 0.46 to 0.31 eV, which may be related to the shallowing of the trap. At the same time, the DOS increased significantly, which means there may be more trap sites in the cellulose and more transport sites may be provided for hopping transport of charges. These two changes both suggested that the charge hopping process could be promoted. The QC calculation provided a new idea for analyzing the origin and a possible tendency of the trap change, but the results were based on a single example of a moisture adsorption site. The specific change of the real cellulose paper is needed to be verified by a more persuasive method.

The TSC method is an effective electrical experimental method to explore the trap characteristics of polymer dielectrics. Thermal stimulation energizes the trapped charge carriers to escape from the trap. The temperature of the current peak is directly related to the energy level of the trap. The TSC results of the cellulose paper with different moisture contents are shown in Fig. 4. Trap current peak 1 was below the temperature of 400 K, corresponding to the trap of the hydroxyl group.

According to the principle of TSC, the trapped charge would be excited by thermal stimulation and escape from the trap, which will form current peaks in the temperature spectrum. The lower the temperature corresponding to the current peak, the lower the thermal stimulation energy required for the charge to escape from the trap, indicating that the trap energy level is lower. As can be seen from Fig. 4, with the increase in moisture content, the trap current peak 1 of the hydroxyl group moved toward the lower temperature direction, so that the corresponding trap energy level decreased. The specific trap energy level of the hydroxyl group was obtained based on Eq. (1), and the trap energy level corresponding to the hydroxyl group decreased from 0.68 to 0.55 eV when the moisture content increased from 0.74% to 4.63%. While the trap energy level decreased, the peak values of TSC increased, which meant that the trap density increased and more charge was involved in trapping and detrapping processes. The changes in experimental TSC results and QC calculation results were consistent. The left shift of the peak in TSC results corresponded to the decrease in the LUMO energy level, and the increase of the peak in the TSC results corresponded to the increase of the DOS. The trap characteristics obtained by TSC were consistent with the above QC-based analysis that the adsorption of moisture on the hydroxyl group changes the trap localized state of cellulose. The presented QC calculations provide a hypothesis on the origin of the moisture-influenced charge conductance process, but it should be noted that the consistency between calculation and experiment is only qualitative, and further verification requires further development of the computational methods and techniques.

**B. The influence of trap on charge transport and conductivity**

1. **The charge transport characteristics in cellulose insulating paper**

The microscopic moisture adsorption decreased the trap energy level, which would influence the macroscopic charge transport process. The polarization and depolarization current (PDC) is an effective method to study the characteristics of charge transport in dielectrics. In Eqs. (2) and (3), $i_a$ is the complete inverse process of $i_p$ contributed by the trapping of charge carriers while the $i'_a$ of $i_d$ is contributed by the de-trapping of charge, and they are opposite transient processes. However, because traps with different energy levels have different effects on charge transport, not all the trapped charges in the polarization process can be de-trapped in the depolarization process where the external electric field is removed. Depending on whether the trapped charges are completely de-trapped during the charge transport process, the transient current mechanism can be divided into two categories and the relation between $i_a$ and $i'_a$ also presents different characteristics, which are summarized in Table I.

When all trapped charges are de-trapped during charge transport, $i'_a$ is the complete inverse process of $i_a$ and they are mirror-symmetrical. In this case, as shown in Eq. (4), the absolute difference $i_p - i_d$ is only the conductance current $i_w$, which is a constant and appears as a flat straight line in the time-domain curve,

$$i_p - i_d = (i_a + i_d) - (i'_a) = i_w. \quad (4)$$

When all trapped charges are not de-trapped during charge transport, only these trapped but not de-trapped charges contribute to $i_a$ and not to $i'_a$, and $i'_a$ is no longer mirror-symmetrical to $i_a$ but is smaller than it. In this case, the result of $i_p - i_d$ includes not only
the steady-state conductance current $i_\sigma$, but also the current contributed by the trapped charge, and the $i_p - i_d$ curve is no longer a flat straight line.

The results of $i_p - i_d$ of cellulose paper with different moisture content are shown in Fig. 5. When the electric field is higher than 1 kV mm$^{-1}$, the charge was injected into the cellulose paper and participated in the transport process.57 As analyzed above, the $i_p - i_d$ results were not a constant and flat straight line due to the trapped charge, and this feature became more significant with the continuous increase in the electric field. Herein, the results under 5 kV mm$^{-1}$ were taken as an example for detailed analysis. After injection into the dielectric, part of the charge was not restricted in the trap and was involved in the charge transport process, forming a conductance current, which is marked by a light blue shadow in Fig. 5. Part of the charge was trapped and cannot be de-trapped without external excitation, and these trapped charges lead to another part of the current, which is marked by a black shadow in Fig. 5. When the moisture content increased, the trap energy level decreased, and the trapped charges were more likely to escape over the trap barrier and participate in the charge transport process. Therefore, as the moisture content of cellulose paper increased, the ratio of current contributed by charge trapping decreased, and the conductance current contributed by charge transport increased, indicating that charge transport was enhanced relative to charge trapping. This charge transport characteristic of the cellulose paper under the influence of moisture is consistent with the accumulation and dissipation characteristics of space charge obtained by the pulse electro-acoustic (PEA) method.57

2. The conductivity mechanism of cellulose insulating paper under the influence of moisture

The conductivity mechanism of amorphous materials and polymer dielectric can be always well explained by the hopping conductance model.27,58 Its visualization is shown in Fig. 6, and the

![Figure 5. The characteristic of charge transport in cellulose paper with different moisture content: (a) 0.74%, (b) 1.82%, (c) 2.97%, and (d) 4.63%. $E$: electric field strength (kV mm$^{-1}$).]
hopping conductivity is determined by the charge hopping between located traps. Based on the Poole–Frenkel effect, the trap potential barrier decreases by $q \lambda E/2$ along the direction of the external electric field, and the probability of hopping transport increases along the same direction as shown in the following equation:

$$\omega_h = \nu \exp \left( -\frac{\phi}{kT} + \frac{q\lambda E}{2kT} \right),$$  \hspace{1cm} (5)

where $\nu$ is the frequency of the thermal vibration, $\phi$ is the trap energy level, $k$ is the Boltzmann constant, $T$ is the Kelvin temperature, $q$ is the charge, $\lambda$ is the distance between two neighboring traps, and $E$ is the external electric field.

When the trap is deep, in other words, the trap energy level is high, the hopping probability is relatively low and the hopping is more likely to occur locally rather than contributing to long-range continuous charge transport. In this case, after hopping, the charge carriers tend to be restricted in the trap, resulting in an uneven distribution of local charges, which was embodied as polarization macroscopically. When the trap becomes shallow with increasing moisture content, the hopping probability becomes relatively high, and more carriers get out of the trap by hopping and participate in long-range continuous charge transport. The long-range continuous charge transport contributes to the hopping conductance, whose current density $j_h$ (or the conductance current $I$) has an exponential relationship with the electric field strength $E$, as shown in the following equation:

$$j_h = 2\nu n \lambda \exp \left( -\frac{\phi}{kT} \right) \exp \left( \frac{q\lambda E}{2kT} \right),$$  \hspace{1cm} (6)

where $j_h$ is the current density and $n$ is the charge carrier density.

The experimental results of conductance current $I$ of cellulose paper varying with $E$ are shown in Fig. 7. When the moisture content was low, $I$ increased with $E$ in an approximately linear trend and the curve was slightly less than linear. When the moisture content was about 3% and higher, $I$ increased exponentially with $E$, which was consistent with the hopping conductance characteristics of Eq. (6). Decreased trap energy level by moisture would enhance the hopping conductance, and the experimental results confirmed this analysis: the higher the moisture content, the more obvious the exponential relationship was, and the conductance mechanism more clearly conformed to the hopping conductance.

From the above analysis, it was clear that the essence of the influence of moisture on the conductivity characteristics was the promotion of the hopping process by a lower trap energy level. More broadly, based on this conclusion, the influence mechanism of temperature and the electric field on the conductivity characteristics of cellulose insulation also became clear. As the temperature increased, the carriers were with higher energy and the hopping probability increased. As the electric field increased, based on the Poole–Frenkel effect, the trap barrier decreased and the hopping probability increased. Both of them were equivalent to the relative shallowing of the trap, and therefore, under high temperature or electric field strength, the relationship between $I$ and $E$ was exponential based on the hopping conductance model. The influence mechanism of temperature and electric field strength on conductance is similar to that of moisture, which further verifies the effective mechanism analysis of the hopping conductance in cellulose insulation in this study.

**IV. CONCLUSIONS**

In summary, this paper aims to reveal the conductivity mechanism under the influence of moisture, integrating microscopic and macroscopic perspectives and employing both computational and experimental research methods. The adsorption characteristics of moisture in cellulose, the change of trap localized states of the hydroxyl group, the corresponding dielectric trap characteristics,
the charge transport characteristics, and the conductivity characteristics were successively studied. Finally, along the above research lines and combining the hopping conductance model, the conductivity characteristics of the cellulose paper influenced by moisture were explained in depth. Specific conclusions are listed as follows:

(1) With the increase in moisture in cellulose, the hydrogen bonds between cellulose and water molecules dominated the increase in total hydrogen bonds, and most of the water molecules were individually adsorbed to the hydroxyl groups by hydrogen bonds. The deteriorating effect of small amounts of moisture on conductivity needs to be considered from factors other than dissolved ions in liquid water.

(2) After the water molecule was adsorbed to the hydroxyl group, besides the LUMO originally on the hydroxyl group, more LUMO appeared on the water molecule, and the corresponding DOS increased. These results indicated that electrons could be trapped more easily, and by the experimental TSC method, it was further verified that the corresponding traps are indeed shallower.

(3) The shallower trap promoted the charges transport process in the cellulose insulation. As the moisture content of cellulose paper increased, the ratio of current contributed by charge transport increased, which indicated that charge transport was enhanced relative to charge trapping.

(4) The promotion effect of moisture on the charge transport led to the conductance mechanism of cellulose insulation to the hopping conductance. As the moisture content increased, more charge carriers escaped from the trap by hopping and participated in long-range continuous charge motion. The current increased exponentially with increasing electric field strength, which conformed to the hopping conductance model.

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AUTHOR DECLARATION

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Haoxiang Zhao: Conceptualization (equal); Data curation (equal); Investigation (equal); Methodology (equal); Software (equal); Writing – original draft (equal). Haibao Mu: Conceptualization (equal); Funding acquisition (equal); Supervision (equal); Writing – review & editing (equal). Daning Zhang: Conceptualization (equal); Funding acquisition (equal); Project administration (equal); Supervision (equal). Björn Baumeier: Software (equal); Writing – review & editing (equal). Huamin Yao: Investigation (equal); Supervision (equal); Writing – review & editing (equal). Guangzi Guo: Data curation (equal); Software (equal); Writing – review & editing (equal). Guanjun Zhang: Supervision (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author on reasonable request.

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