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Solvent-molecule interaction induced gating of charge transport through single-molecule junctions

Zheng Tang,‡[1] Songjun Hou,‡[2] Qingqing Wu,‡[2] Zhibing Tan,‡[1] Jueting Zheng,[1] Ruihao Li,[1] Junyang Liu,[1] Yang Yang,[1] Hatef Sadeghi,[2] Jia Shi,[1] Iain Grace,[2] Colin J. Lambert,[2],* and Wenjing Hong[1],*

1 State Key Laboratory of Physical Chemistry of Solid Surfaces, Collaborative Innovation Center of Chemistry for Energy Materials (iChEM), College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China
2 Department of Physics, Lancaster University, Lancaster LA1 4YB, UK

‡These authors contributed equally to this study.
* Correspondence author: whong@xmu.edu.cn, c.lambert@lancaster.ac.uk

Abstract To explore solvent gating of single-molecule electrical conductance due to solvent-molecule interactions, charge transport through single-molecule junctions with different anchoring groups in various solvent environments was measured by using the mechanically controllable break junction technique. We found that the conductance of single-molecule junctions can be tuned by nearly an order of magnitude by varying the polarity of solvent. Furthermore, gating efficiency due to solvent–molecule interactions was found to be dependent on the choice of the anchor group. Theoretical calculations revealed that the polar solvent shifted the molecular-orbital energies, based on the coupling strength of the anchor groups. For weakly coupled molecular junctions, the polar solvent–molecule interaction was observed to reduce the energy gap between the molecular orbital and the Fermi level of the electrode and shifted the molecular orbitals. This resulted in a more significant gating effect than that of the strongly coupled molecules. This study suggested that solvent–molecule interaction can significantly affect the charge transport through single-molecule junctions.

1 Introduction

Wiring functional molecules into electrical circuits has been found to have significant potential for miniaturisation of electronic devices [1-6]. Various intrinsic molecular factors have been investigated to advance the understanding on their effect on single-molecule junction conductance, such as conformation [7-9], anchor groups [10, 11], electrodes [12], hybridisation [13], and quantum interference [14-16]. By altering these parameters, molecular switching can be achieved due to changing redox states [17-19], protonation [20, 21], and connectivity [3]; however, the molecular states have been restricted to be less than three. Electrochemical and electrostatic gating [22, 23] have also been found as promising approaches for tuning the energy level alignment, although the additional gate electrode has been found to bring technical challenges for the integration. To address this issue, solvent gating has been considered

a potentially simple method for continuously fine-tuning the charge transport through single-molecule junction with multiple accessible states, although previous studies have reported a relatively smaller gating effect [24].

Gating of the charge transport, through molecular junctions typically occurs through electrostatic interaction [11, 22]. Several mechanisms have been proposed in existing literature on the solvent effects, such as solvent binding to the functional groups in the molecular backbone [25], solvent binding to the molecular backbone [26], solvent binding to the gold electrodes [24, 27], and protonation tuning of the molecules induced by the solvent [20]. A few recent studies demonstrated a highly efficient charge transport through supramolecular interactions [28], suggesting that the electrostatic interactions between the solvent and molecule can be effectively used to tune the charge transport through single-molecule junctions.

2 Experimental

In this study, we demonstrated that solvent-molecule interaction resulted in a significant solvent gating effect in charge transport through single-molecule junctions, created using the mechanically controllable break junction (MCBJ) technique [29, 30]. Oligophenylethynylene-sulfurmethyl (OPE-SMe) and its derivatives were employed to form single-molecule junctions [31, 32]. A mixture of 20 vol% tetrahydrofuran (THF) and 80 vol% 1,3,5-trimethylbenzene (TMB) was selected as the prototype solvent for the single-molecule conductance measurement (THF for solubility and TMB for stability and low permittivity, see SI section 1.1 for detailed discussion on the influence of different solvents in single-molecule conductance measurement) [33]. The conductance measurements of the target molecules in different solvents were conducted using the MCBJ technique (as shown in Scheme 1). Results demonstrated that the conductance of OPE-SMe can be regulated to an order of magnitude higher by adjusting the solvent environment. This solvent effect was further investigated by varying the anchoring groups of the molecular junctions and solvent molecules.
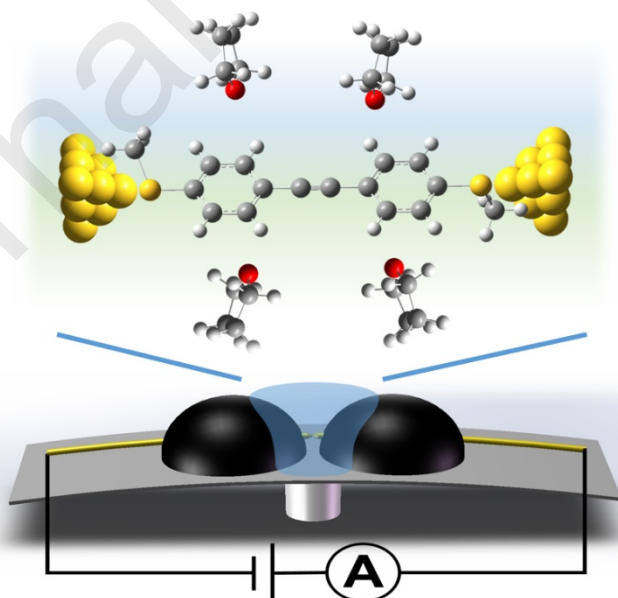
Scheme 1 (Color online) Schematic of MCBJ configuration and single-molecule junction with solvent molecules.

3 Results and discussion

We used pure THF and TMB to prepare a 0.01 mmol/L solution of OPE-SMe, separately. In each case, conductance-displacement traces (as shown in Fig. 1a) were continuously recorded. The individual traces showed variation in the conductance as a function of distance during the process of breaking a single-molecule junction. After a short plateau at the conductance quantum (G_0, which equals $2e^2/h$, 77.6×10^3 nS), which marked the single-atomic contact of Au-Au, the conductance trace was observed to rapidly drop to the plateau of the molecular conductance and went to the tunnelling background afterwards. The one-dimensional (1D) conductance histograms, shown in Fig. 1b, constructed from ~1000 such traces, showed the conductance peaks that indicated the most probable junction conductance. The conductance of OPE-SMe, determined from the Gaussian fitting of the conductance peak, was observed to peak at $10^{-2.1}$ and $10^{-3.0}$ G_0 (616.4 and 77.6 nS) in THF and TMB, respectively, which showed high solvent-dependence. To confirm that conductance of single-molecule junctions were measured, we constructed two-dimensional (2D) conductance-displacement histograms (Fig. 1c and d). The dashed circles represent the overlapped area of the molecular plateaus [21]. Insets of Fig. 1c and d showed the displacement distribution analysis of the molecular plateaus [34], suggesting that the configurations of OPE-SMe junctions were stable and fully elongated in the solvents.
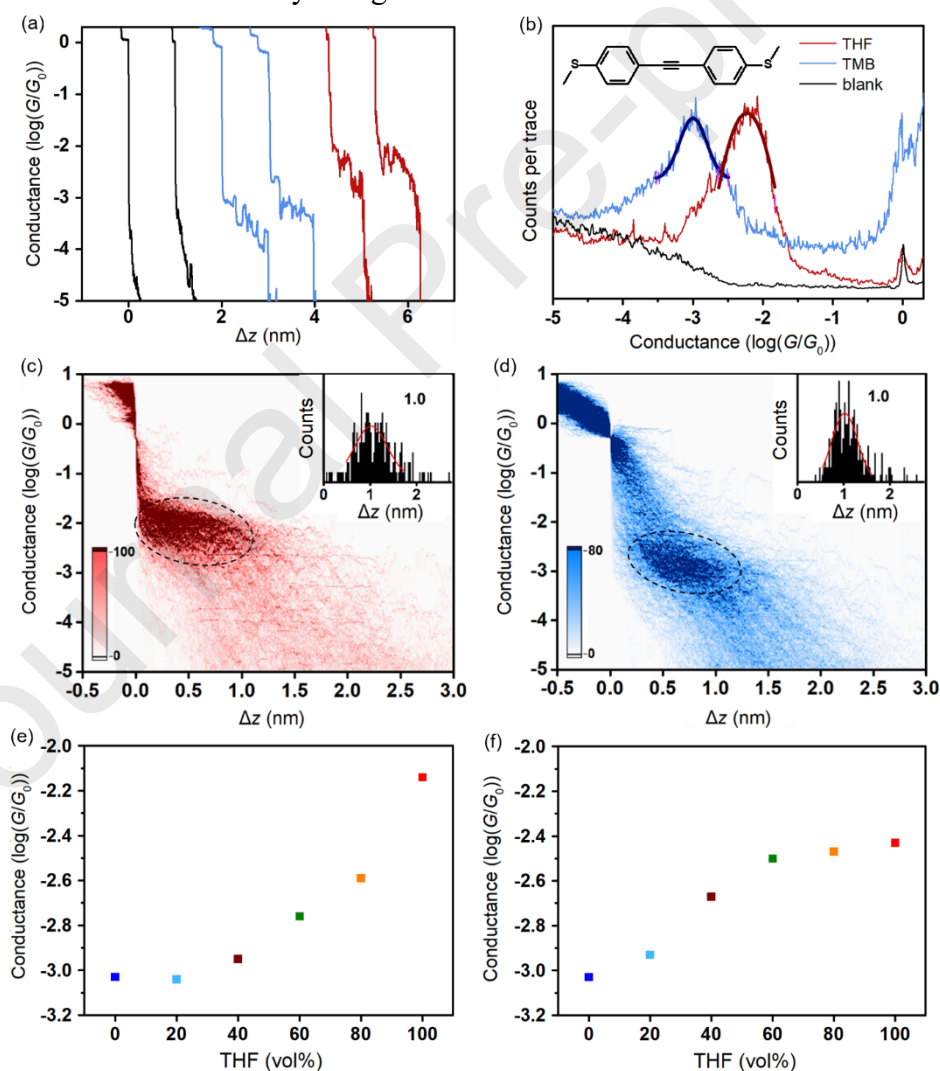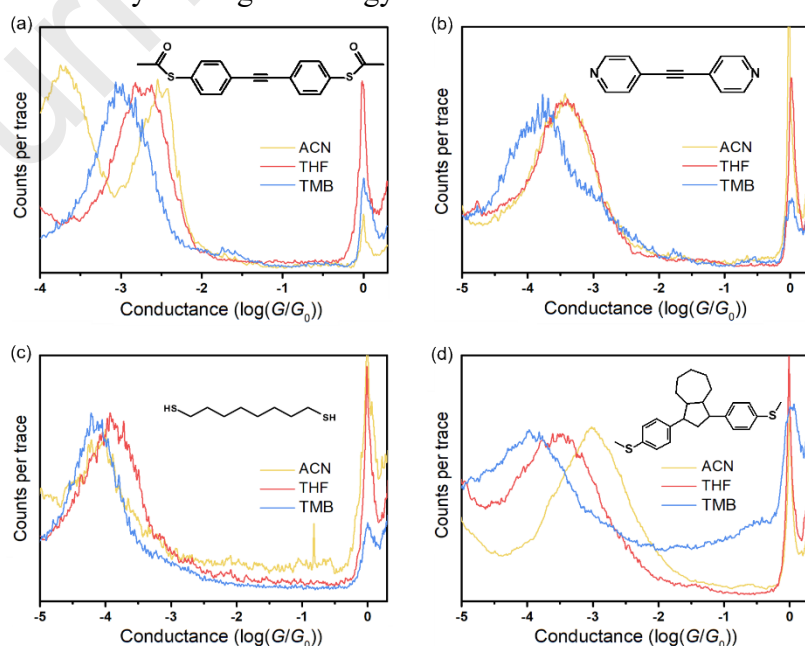

Fig. 1. (Color online) (a) Typical individual conductance-displacement traces of pure TMB (black) and OPE-SMe junctions in different solvents (blue and red lines represent TMB and THF, respectively), (b) 1D conductance histograms of pure TMB and OPE-

SMe junctions in different solvents from ~1000 traces without data selection. 2D conductance-displacement histograms constructed from ~1000 traces for OPE-SMe in (c) THF and (d) TMB. Inset: Relative displacement distribution histograms, (e) conductance values of OPE-SMe in the corresponding mixed solvents (THF:TMB (v:v) = 0:1 (blue), 1:4 (light blue), 2:3 (wine), 3:2 (olive), 4:1 (orange) and 1:0 (red)), (f) conductance values of OPE-SMe in the corresponding mixed solvents (ACN:TMB (v:v) = 0:1 (blue), 1:4 (light blue), 2:3 (wine), 3:2 (olive), 4:1 (orange) and 1:0 (red)).

To further verify the effect of solvents on the charge transport of molecular junctions, conductances of OPE-SMe in various volume ratios of THF and TMB were measured. Mixed solvents with different ratios were used to gradually vary the polar environments of the system. As shown in Fig. 1e, the single-molecule conductance of OPE-SMe depended on the content of THF in the mixed solvents. In addition, such dependence of this solvent was found in another common polar solvent (acetonitrile/ACN), as shown in Fig. 1f (detailed conductance data are shown in Figs. S2–S10 online), which indicated that the increase in the solvent polarity can significantly improve the charge transport of the molecular junctions.

To explore the mechanism of solvent gating on the charge transport, control experiments were carried out with oligophenylethynylene-sulfuracetyl (OPE-SAc), oligoaryleneethynylene (OAE), 1,8-octanedithiol (ODT) and 1,3-azulene (1,3Az) [2, 34-37]. Results from the conductance measurements for OPE-SAc, OAE and ODT in different solvents are shown in Fig. 2a, 2b and 2c. When compared with the results of other studies ($G_{OPE-SAc} = 10^{-3.0}$ $G_0 = 77.6$ nS, $G_{OAE} = 10^{-3.6}$ $G_0 = 19.5$ nS, $G_{ODT} = 10^{-3.6}$ $G_0 = 19.5$ nS and $G_{1,3Az} = 10^{-3.8}$ $G_0 = 12.3$ nS), the single-molecule conductances of OPE-SAc, OAE and ODT did not exhibit a significant solvent induced shift, while that of 1,3Az was observed to be manipulated by the solvent in the single-molecule conductance measurement (see Figs. S11–S14 online for details). Thus, we hypothesised that the solvent effect on the molecular junctions depends on the nature of the anchor groups. As no functional groups were found on the OPE-SMe backbone for THF or TMB to form a chemical bond, and interactions between the solvents and gold atoms were too weak to affect the contact work function [24, 25]. Electrostatic interactions were considered to play a dominant role in gating the conductance of molecular junctions by shifting the energy of the frontier molecular orbitals.

Fig. 2. (Color online) (a) 1D conductance histograms of OPE-SAc, (b) OAE, (c) ODT and (d) 1,3Az in different solvents (blue, red and yellow lines represent TMB, THF and ACN, respectively) from ~1000 individual conductance-displacement traces. Insets represent the corresponding molecular structure.

To further examine the response of conductance to different solvent molecules, transmission spectra $T(E)$ were calculated by combining the DFT package SIESTA with the quantum transport code Gollum (see the Supplementary materials Section 2 for detailed method) [38, 39]. The relaxed molecules, OPE, OAE and ODT, measured in the experiment were attached to the gold electrodes and were surrounded by different solvents: THF, ACN or TMB. For the solvent molecules, with an electric dipole moment (e.g., THF and ACN), we constructed conformations with dipole moment pointing towards or away from the backbone molecule, as shown in Fig. 3a and b, which showed the examples of OPE-SMe with two THF molecules (additional backbone molecules with other solvent molecules are shown in the Supplementary materials). For solvent molecules without an electric dipole moment (e.g., TMB), we selected two configurations: TMB being parallel or perpendicular to the backbone, as shown in Fig. S16b (online).
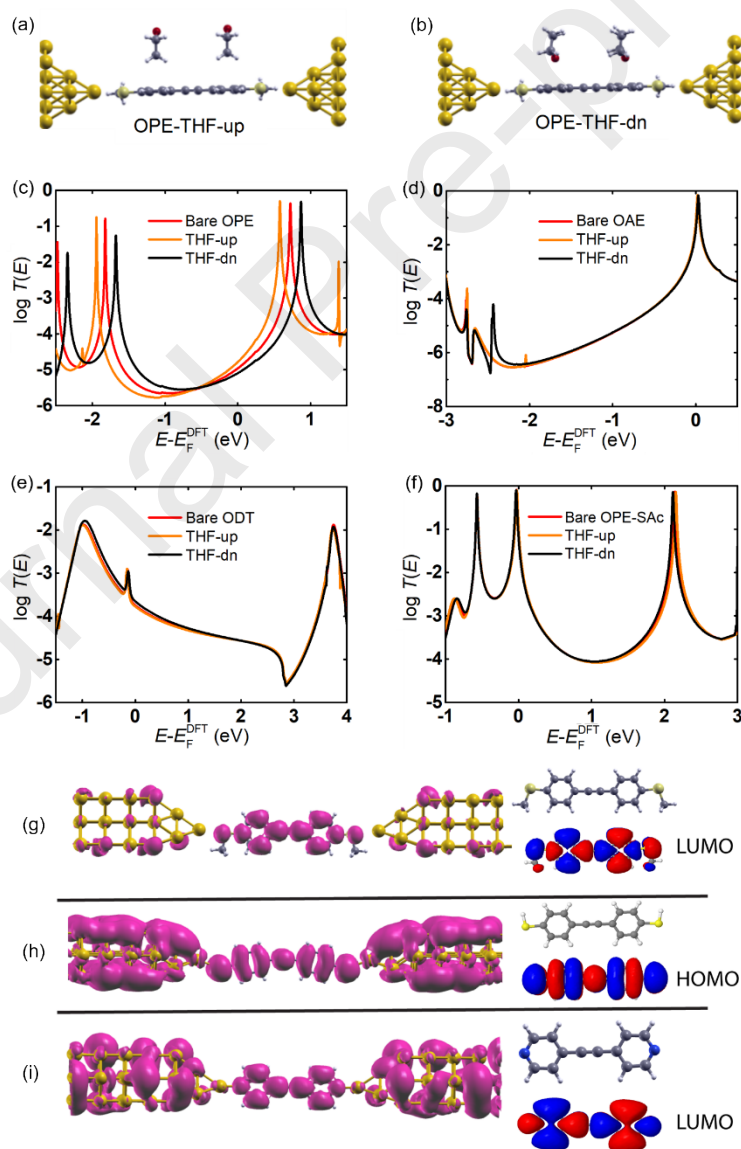
Fig. 3. (Color online) (a) Conformation for OPE-SMe with two THF molecules pointing outward, named "THF-up", (b) conformation for OPE-SMe with two THF molecules pointing inward, named "THF-dn". The transmission coefficient $T(E)$ vs. electron energy for (c) OPE-SMe, (d) OAE, (e) ODT and (f) OPE-SAc with or without the two THF molecules. For the case with THF molecules, the conformation was observed to be similar to (a) and (b), (g) LDOS (left) with the magenta colour in the energy window of 0.1 eV, around the LUMO resonance peak and isolated OPE-SMe molecule as well as the corresponding LUMO (right) and for (h) OPE-SAc and (i) OAE.

To explore the role of anchor groups in the presence of polarised solvent molecule, backbone molecules were fixed during the optimisation process, while the solvent molecules were allowed to relax. Results for THF are shown in Fig. 3 (see Figs. S16–S19 (online) for other backbone molecules). For OPE-SMe, when the oxygen-side of a THF solvent molecule was close to the backbone, the transmission curve was observed to shift to a higher energy (black line in Fig. 3c). In contrast, when the other end of the solvent molecule moved closer to it, the transmission curve was observed to shift to a lower energy (orange line in Fig. 3c). The two opposite shifts of the transmission function were attributed to different gating effects due to the orientation of the solvent, whose dipole moment pointed from the positive to the negative oxygen-side. However, as shown in Fig. 3d–f, for the backbone molecules OAE, ODT and OPE-SAc with solvent, their transmission functions were observed to barely change over a large energy range near the DFT-predicted Fermi energy. Similar shifting trends in the transmission function of the three backbone molecules were observed in the solvent ACN (see Figs. S16–S19 online).

The only difference observed between OPE-SMe and OPE-SAc was their anchor groups, which indicated that the anchor groups played a dominant role in determining the effectiveness of the solvent gating. To gain further insight into the origin of these gating effects, local density states (LDOS) around lowest unoccupied molecular orbital (LUMO), highest occupied molecular orbital (HOMO) and LUMO resonances for OPE, with anchor groups -SMe, -SAc and OAE with pyridyl anchoring groups embedded in the junction were examined, as shown in Fig. 3g–i. For anchor groups -SMe, LDOS was observed to be mainly localised on the OPE backbone, while either HOMO of anchor groups -SAc or LUMO of pyridyl anchor groups were observed to be distributed almost equally on the gold electrodes as well as on the backbone molecule (these features were also observed in the wave functions shown in Figs. S20 and S21 online). In this case, the gold and molecule were observed to be more strongly coupled and less likely to be influenced by the gating effect of the solvent. The sensitivity of the molecular orbital energy to a local perturbation, such as a solvent molecule, can be explained by the perturbation theory, which predicts that the energy shift is $\Delta E = \langle \phi_n | H' | \phi_n \rangle$, where ϕ_n is the nth molecular orbital and H' is the perturbation. If this normalised orbital is extended over N atomic pi orbitals, then its amplitude on any pi orbital is $(\sim 1/\sqrt{N})$. If the local perturbation (H') acts over M such sites, then the shift in the orbital energy ΔE will be proportional to M/N. Consequently, if N is large, ΔE would be relatively smaller, whereas, the effect would be larger for a more localised molecular orbital spread over a smaller number of sites N. This mechanism is significantly different from that mentioned in our previous work [25], where a shift in the gold contact work function was induced by solvent binding to the undercoordinated Au sites. Such a shift in the gold work function was found to be independent of the nature of the anchors.

After discussing the importance of the anchor groups on solvent gating, we will next discuss the influence of different solvents on the backbone, by taking OPE-SMe as an example. For TMB, no influence on OPE was observed in the parallel case, while a small shift was observed to appear for the standing case due to slightly positively charged H in the methyl group (see Fig. S16d online). Owing to this, we only consider the influence of THF and ACN in this section. To simulate the real experiment, 112 configurations were constructed each for OPE with one THF molecule and one ACN molecule. These curves are shown in Fig. 4a and 4b. Although the transmission curves could shift towards both higher and lower energies, more curves were observed to shift towards lower energies, indicating an increasing trend in the conductance when the OPE molecule was placed in a polar solvent. This was attributed to the negatively charged carbon atoms in the two phenyl rings of OPE, which attracted the positive part of the solvent molecule. These results can be clearly observed in Fig. 4c2 and 4c4, where more than 70% of the total configurations exhibited an increasing trend, which was observed to be consistent with the experimental results. For ACN, a larger conductance range is shown in Fig. 4c, and the conductance variations were also observed to be more sensitive to the orientation and movement of ACN, which were all attributed to the greater electric dipole momentum than that of THF. Since it is exorbitantly expensive to computationally simulate all the surrounding solvent molecules, we investigated the influence of the solvent molecules by placing just one molecule in 112 different relaxed configurations, which allowed us to collect the data [18, 25, 26].
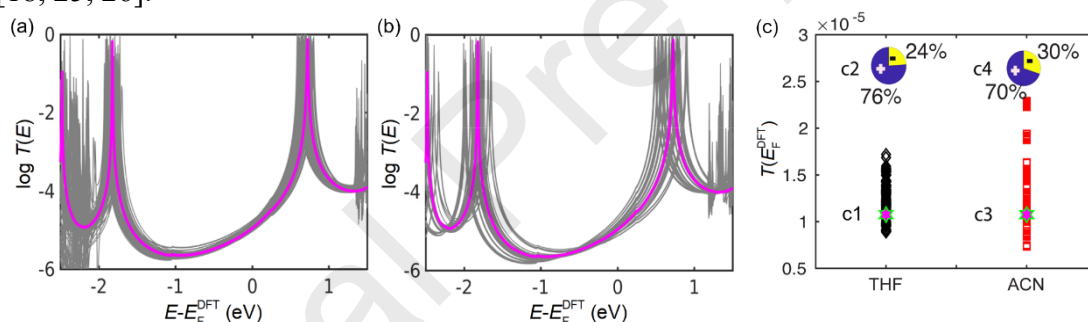
Fig. 4. (Color online) Transmission curves of 112 configurations (see the Supplementary materials for details) for OPE with one solvent molecule ((a) THF and (b) ACN), the magenta and grey curves represent bare OPE and OPE in solvent, respectively. The statistical results, with transmission coefficient at the DFT-predicted Fermi energy level, are shown in (c), where the magenta hexagonal stars, black diamonds and red squares represent bare OPE, OPE with (c1) one THF and (c3) OPE with one ACN, respectively. The plus and minus signs imply increase and decrease in the conductance, respectively.

4 Conclusions

In this study, we proposed an efficient gating approach for fine-tuning single-molecule conductance by controlling the solvent-molecule interaction. Results showed that the conductance of the molecular wires, which weakly coupled to the electrodes, can be varied by up to 800% by adjusting the polarity of the environment. Theoretical calculations revealed that the solvents influenced the molecular orbital energies and coupling strength of the anchoring groups, and electrodes controlled the magnitude of the shift. This study demonstrated that solvent-molecule interactions can provide a highly efficient gating approach to control the charge transport in single-molecule devices.

Conflict of interest

The authors declare that they have no conflict of interest.

Author contributions

Wenjing Hong, Colin J. Lambert, Zheng Tang and Zhibing Tan originally convinced the idea and designed the experiments. Zheng Tang carried out the break junction experiments and analyzed the data. Zheng Tang and Songjun Hou wrote the manuscript with input from all authors. Wenjing Hong, Ruihao Li and Jia Shi built the electrical measurement instrument and wrote the software to control the break junction setup. Zhibing Tan, Junyang Liu, Jueting Zheng and Yang Yang revised the manuscript. Songjun Hou, Qingqing Wu, Hatef Sadeghi, Iain Grace and Colin J. Lambert performed the theoretical modeling. All authors conceived the work and discussed the experiments.

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Zheng Tang received his B.S. degree in 2016 from the College of Chemical Engineering, Beijing University of Chemical Technology. He joined the research group of Prof. Wenjing Hong in the College of Chemistry and Chemical Engineering, Xiamen University, as a graduate student. His research is mainly focused on single-molecule electronics and precise instrument.

Songjun Hou is currently a postdoctoral researcher in the Department of Physics, Lancaster University, with Prof. Colin Lambert. He received his Ph.D. degree in 2019 from the Department of Physics, Lancaster University, with Prof. Colin Lambert. His research is focused on the quantum transport in single-molecule devices.

Qingqing Wu is currently a research associate in the Department of Physics, Lancaster University, with Prof. Colin Lambert. She received her Ph.D. degree in 2018 from the Department of Physics, Lancaster University, with Prof. Colin Lambert. Her research interest is focused on the molecular electronics and photon catalysis.

Zhibing Tan received his Ph.D. degree in 2019 from the Department of chemical engineering, Xiamen University, China, under the supervision of Prof. Wenjing Hong. He is currently a postdoctoral researcher with Prof. Wenjing Hong. His research is focused on charge transport through supramolecular interaction at the single-molecule level.

Prof. Colin Lambert received his Ph.D. degree in 1979 from the University of Hull in UK. He joined Lancaster University in 1983 and was awarded a Professorship in 1990. His research interests include theory of quantum transport in nanostructures and single-molecule junctions and in related areas.

Wenjing Hong received his Ph.D. degree in 2013 from the University of Bern in Switzerland. In 2015, he became a full professor at Xiamen University, China. His research interests include single-molecule electronics, scientific instruments, and artificial intelligence.