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SPECIAL ISSUE: Celebrating the 130th Anniversary of Tianjin University

Trace-level oxygen doping in organic semiconductors: mechanistic insights and precise modulations

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Organic semiconductors (OSCs) are showing great promise in large-area wearable devices, optoelectronic displays, logic circuits, and next-generation optoelectronic applications [1–9]. Examples include organic field-effect transistors (OFETs), organic light-emitting diodes (OLEDs), organic photovoltaic cells (OPVs), and sensing devices. However, OSCs encounter significant challenges in widespread commercialization [10–13]. Compared with their inorganic counterparts connected by strong covalent bonds, the structural characteristics of OSCs films are predominantly governed by van der Waals interactions [14–19], rendering their optoelectronic properties typically dependent on the synergistic effects between intrinsic properties and extrinsic effects, such as impurities and defects [20–26].

Ubiquitous oxygen represents one of the most prevalent extrinsic impurities readily encountered in OSCs. Owing to its high electronegativity, oxygen demonstrates a strong propensity toward redox interactions within OSCs. Oxygen doping has gained great interest in organic electronic community, involving its effects on charge transporting and applications in devices [27–35]. For a long time, oxygen has been considered a charge-carrier trap that heavily deteriorates performance and stability. Consequently, researchers have predominantly focused on developing strategies to suppress oxygen incorporation and mitigate its detrimental effects in OSC systems [20,35–37]. In recent years, quite different viewpoints have emerged that oxygen doping shows a completely opposite effect at trace level, i.e., trace oxygen improves the performance and stability of organic electronic devices by pre-emptying the electrons from the donor-like traps [38]. And some strategies have been developed to modulate oxygen doping at trace level, achieving optimized device mobility and stability [38–43].

Although significant progress has been made in this research field, the oxygen doping mechanism and its effect on optoelectronic devices are not yet fully understood. An important research direction is to address the fundamental challenges associated with understanding oxygen doping mechanisms in OSCs, coupled with the development of targeted modulation strategies.

Herein, this perspective delineates the mechanistic underpinnings of trace oxygen doping phenomena in OSCs, discussing the state-of-the-art modulation strategies to enhance device performance. Through systematic analysis of structure-property relationships, we discuss oxygen relevant modifications in charge transport dynamics and operational reliability of organic electronic devices. Building on this foundation, the perspective proposes a development framework for oxygen element doping engineering while outlining emergent challenges in interfacial stabilization protocols.

MECHANISTIC INSIGHTS OF TRACE OXYGEN DOPING IN OCSs

OSCs are essential components in OFET devices, governing their performance and stability [44–50]. The presence of extrinsic impurities substantially accelerates the performance deterioration of OSCs during device operation and ambient exposure. Among the many involuntary introduced extrinsic factors, ubiquitous environmental oxygen molecules readily permeate both the OSCs bulk and their interface with the dielectric layer, owing to their high electron affinities and small molecular volume [51–56]. They are regarded as the most common causes of charge-carrier traps in many OSCs, critically deteriorating device performance [57–64]. Zhang's group [27] observed that prolonged air exposure of the device led to adsorption and gradual penetration of oxygen molecules into the organic semiconductor channel. These traps minority electrons injected under positive gate bias, thereby leading to non-ideal device characteristics. A novel method for analyzing trap states in semiconducting molecular crystals is introduced by Podzorov's group [35]. Their studies revealed that exposure to oxygen and subsequent oxygen diffusion result in the creation of oxygen-induced trap states, which significantly decreases both dark conductivity and photoconductivity of rubrene by over tenfold. Photo-oxidative degradation occurs when OSCs undergo chemical structural changes exposured to light (mainly UV-visible) and oxygen that breaks conjugated π-systems. It disrupts charge transport pathways and decreases conductivity [65–67]. An antioxidant strategy based on nickel chelate ($Ni(dtc)_2$) with the addition of 2–10 wt% of $Ni(dtc)_2$ was proposed by Brabec's

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group [67], which can significantly retard the photobleaching rate of the films by both sacrificial and non-sacrificial mechanisms. This strategy effectively inhibited the photo-oxidative degradation of conjugated polymers and their fullerene blend systems. Durrant *et al.* [52] compared the photochemical stability of two donor polymers in neat and blend films. They employed transient absorption measurements and a molecular singlet oxygen indicator to demonstrate that the polymer with the higher yield of long-lived triplets exhibits higher yields of photochemical single oxygen in both neat films and blend films.

Previous understanding of oxygen effects experimentally relies on the conventional deoxygenation methods [28,67–69], e.g., annealing and sublimation. Very recently, it is reported that trace-level oxygen is still presented in the majority of the purified OSCs [38], implying that trace oxygen residues are unavoidable in these processes. Some reports demonstrated that this trace oxygen molecules have positive impacts on OSCs by optimizing conductivity, passivating defects, and morphological control via crystallization kinetics [27,38–43]. Zhang *et al.* [27] found that moderate exposure to ambient air (containing H_2O and O_2 molecules) can effectively induce doping in organic materials at the electrode interface, passivating defect states generated during electrode deposition, thereby enhancing charge carrier injection efficiency and improving the ideality of device performance. Havinga's group [42] revealed that pristine tetracyanoquinodimethane (TCNQ) films demonstrated minimal switching characteristics. However, following ambient air exposure over time, these films exhibited a remarkable enhancement in switching performance, achieving a switching ratio of three orders of magnitude.

Huang *et al.* [38] discovered that trace oxygen (~10^{15} cm^{-3}) is inherently presented in a wide range of OSCs even after rigorous purification (Fig. 1) by *quasi-in-situ* ultraviolet photoelectron spectroscopy (UPS), the time of flight secondary ion mass spectrometry (TOF-SIMS) and electron paramagnetic resonance spectroscopy (EPR). This residual oxygen interacts with OSCs, forming superoxide anion radicals (O_2^-) and organic radical cations (ORCs). The authors developed an effective de-doping method (i.e., deoxygenation) based on soft plasma and a re-doping method by illumination in oxygen. The p-type properties of OSCs gradually disappeared during the de-doping process and reversed under the re-doping process. It indicates that oxygen is the origin of the p-type transport behaviour of OSCs. This insight is completely opposite to the previously reported carrier trapping and can clarify some previously unexplained organic electronics phenomena. This work expands the explorable property space of organic semiconductor materials, opening new avenues for investigating their intrinsic optoelectronic

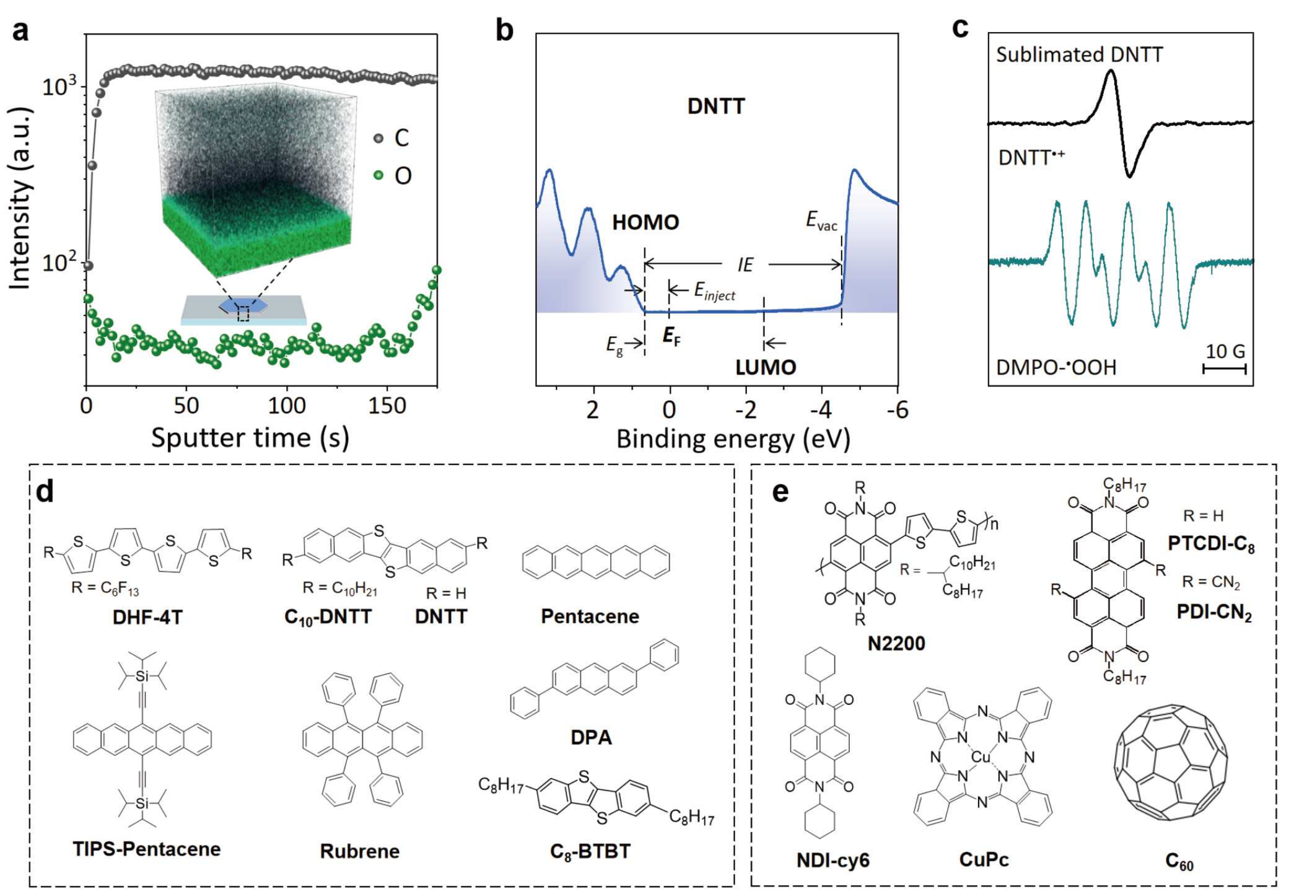

Figure 1 (a) Intensity of the TOF-SIMS data for the C and O elements of the fresh DNTT single crystal. Inset is the 3D reconstruction of the depth profile. (b) Valence photoemission spectrum and secondary electron spectrum extracted from the UPS measurement of the fresh DNTT film. Ionization energy (IE), vacuum level (E_{vac}), and injection barrier (E_{inject}) are exacted from the UPS result, and the energy gap (E_g) is obtained from the UV-vis absorption spectrum. The energy position of the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital(LUMO), and the Fermi level (E_F) are thus determined. (c) EPR signals of ORCs and DMPO-•OOH (the adduct of DMPO with O_2^-) in fresh DNTT film, suggesting the innate oxygen doping in OSCs. Different OSCs of (d) p-type and (e) n-type. Reprinted with permission from Ref. [38]. Copyright 2024, Springer Nature.

properties and controllable doping.

MODULATING STRATEGIES FOR ELECTRONIC PROPERTIES OF OSC AND DEVICES

Building upon the mechanistic insights into oxygen doping and its pivotal role in OSCs, innovative strategies for trace oxygen modulation were presented, providing guidelines for leveraging oxygen as a tuneable functional component in OSCs and device design. It is conducive to addressing challenges related to long-term stability and reproducibility. Neher's group [36] blended poly(3-hexylthiophene) (P3HT) with polystyrene (PS) at a ratio of 0.05/0.95, spin-coated the blends on substrate in a nitrogen glovebox ($O_2/H_2O \leqslant 1$ ppm), and subsequently annealed the blends under vacuum. This process significantly enhanced the blends performance. They attributed the improved stability to the "encapsulation" effect of the insulating PS matrix on P3HT, which effectively suppresses oxygen penetration into the semiconducting polymer. Jurchescu *et al.* [37] identified the most probable and severe degradation pathways in organic transistors by real-time monitoring of trap density of states (DOS), guided by density functional theory (DFT) calculations during device operation, and they devised the most efficient packaging strategy for each type of device, resulting in high-performance, environmentally and operationally stable small molecule and polymer transistors. However, the conventional annealing and encapsulation strategies do not effectively address the aforementioned stability issues induced by the "inherent" trace oxygen.

The soft plasma treatment and photo-oxygen synergistic technique were used to precisely control the oxygen doping in OSCs and devices. A nondestructive soft plasma treatment (H_2, N_2 or Ar) was developed by Huang *et al.* [38] to remove trace-level oxygen (i.e., de-doping) in OSCs. To achieve reversible oxygen doping/de-doping processes, the researchers also developed a light-oxygen synergistic technique for oxygen re-doping: exposing the de-doped organic devices to light of specific wavelengths under an O_2 atmosphere, which enables the controllable oxygen adsorption and charge transfer. Based on this strategy, OFETs no matter with negative threshold voltage (V_T) or positive V_T could be modulated to turn on at approximately 0 V, without the observed decrease in mobility. And the conductivity of C_{10}-DNTT could be tuned in a large range. Attractively, the polar type of the transport behaviors can be modulated by this de-doping and re-doping strategy. For example, OFETs of TIPS-pentacene show p-type behavior both in air and vacuum, but they can be modulated to be n-type via our de-doping process, and certainly can be recover to p-type again by our re-doping process. In addition, it is well known that the N2200 is a high-performance n-type OSC, which can be endowed with p-type behavior via the re-doping strategy, and certainly can be converted to n-type again by de-doping process.

It is widely recognized that O_2 introduces defects into OSCs, degrading OFET performance [70–72], suggesting that high-purity inert gases (Ar, N_2) should be used as carrier gases during OSC crystal growth. However, Sun *et al.* [40] developed an oxygen-induced lattice strain (OILS) strategy by originally introducing oxygen into OSC crystals to generate lattice strain in the growth process. Lattice compression in OSC crystals induces closer π-π stacking distances, which increases frontier orbital overlap and strengthens intermolecular charge transfer integrals. These synergistic effects notably improve the electrical performance and stability of the OSCs crystal. The contact resistance is lowered to 25.5 kΩ cm, while the maximum mobility soars up to 15.3 $cm^2\,V^{-1}\,s^{-1}$ in the OILS DNTT crystal. To fully elucidate the impact of lattice strain on the morphological stability of OSC crystals, the authors transferred both OILS DNTT crystals and strain-free DNTT crystals onto identical SiO_2/Si substrates for *in-situ* investigation of the morphological stability of DNTT crystals under high temperatures. After annealing at 160 °C for 5 min, the strain-free DNTT crystals exhibited severe cracking, degradation, and destruction, whereas the OILS DNTT crystals maintained excellent crystalline morphology. This demonstrates a significant enhancement in the morphological stability of OILS DNTT crystals. This work builds an important bridge between microstructure and material properties, providing new insights for developing high-mobility and high-stability OFETs.

The high contact resistance (R_c) at metal/semiconductor nanointerfaces significantly limits device integration and miniaturization by reducing charge injection/extraction efficiency and exacerbating power dissipation. Conventional approaches struggle to simultaneously achieve strong orbital coupling and low Schottky barrier height. Fu *et al.* [41] developed an oxygen-induced nanointerface engineering strategy to lower the electrode-OSC energy barrier through controlled oxygen and achieved an ultralow channel width-normalized R_c ($R_c{\cdot}W$) of 89.8 kΩ cm and a high mobility of 11.32 $cm^2\,V^{-1}\,s^{-1}$. This approach effectively reduces the contact resistance and the metal-semiconductor interface barrier height, leading to a remarkable enhancement in charge carrier mobility.

For n-type OSCs, oxygen doping, whether in trace amounts or in large quantities, has a negative impact. n-type OSCs encounter key challenges such as poor reliability, low performance, and a limited material pool, with electron transport instability being the fundamental cause [23,73–75]. These challenges are largely due to chemical degradation and electron trapping induced by external oxidizing agents [23,51–56]. Although n-type OSCs can be designed to have high electron affinity to improve their anti-oxidative properties, organic radical anions generated during device operation are thermodynamically unstable and easily react with oxygen and water, especially reactive oxygen species (ROS) [76–78], leading to the low stability of n-type OSCs and their electronic devices. Yuan *et al.* [39] have developed a general strategy using vitamin C (VC) to scavenge ROS that significantly improve the stability of n-type OSCs and their device performance, for example, OFET (Fig. 2). The researchers discovered that spin-coating VC onto the surface of PTCDI-C_8 (a typical n-type organic semiconductor molecule, Fig. 1e) thin films can significantly reduce their photo-oxidation rate and markedly enhance the material's oxidative stability. Subsequently, the research team employed OFETs as model devices to explore the application of VC on organic electronics. To suppress VC crystallization, the researchers blended VC with polyurethane (PU) and spin-coated the mixture onto OFETs based on nine different n-type molecular semiconductor. Compared to pristine devices, all VC-PU-treated OFETs exhibited substantial performance enhancements, with electron mobility improvements reaching up to 38-fold. The operational stability and photo-oxidation resistance of n-type OFETs were significantly enhanced, with the superior device performance maintained in air for over 255 days.

The author found that VC scavenges reactive oxygen species and inhibits their generation by sacrificial oxidation and non-sacrificial triplet quenching in a cascade process, which not only

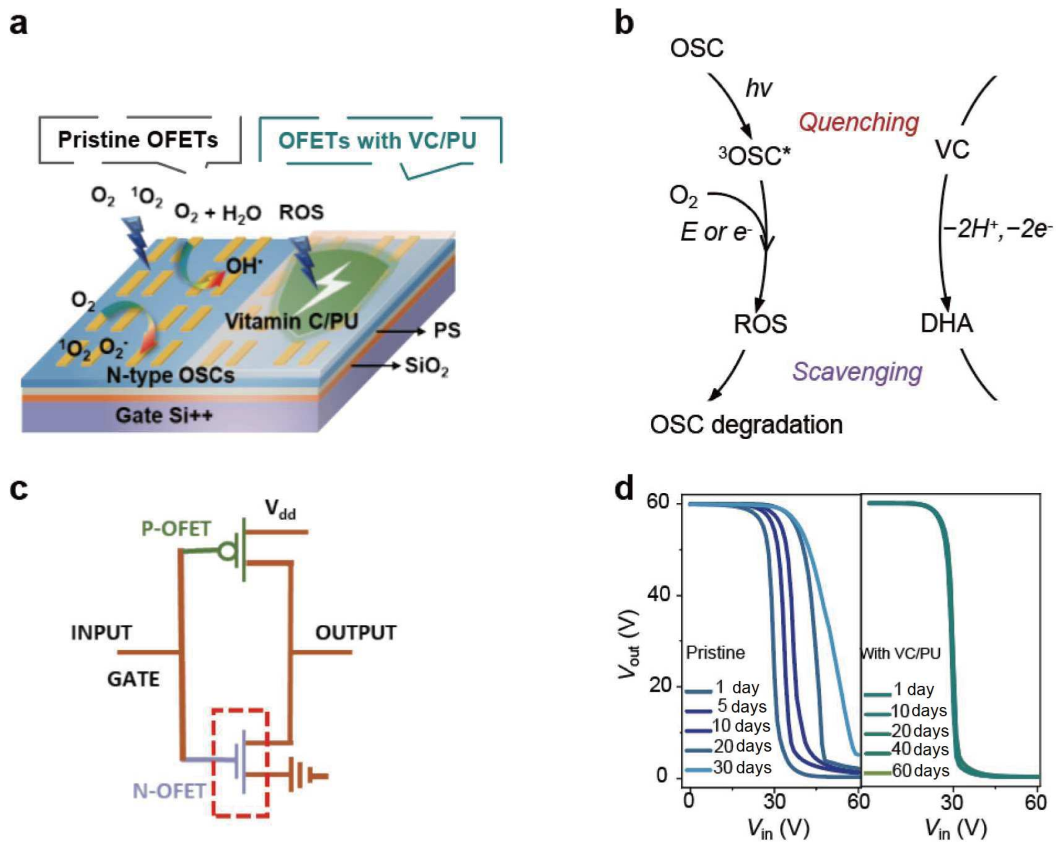

Figure 2 (a) Schematic diagram of OFETs with and without VC–PU protection. (b) Diagram of the stabilization mechanism. (c) Schematic of organic complementary inverters. The dotted red line marks the n-channel OFET (N-OFET) part covered by VC–PU. (d) Static voltage transfer curves of inverters with and without VC–PU at $V_{dd} = 60$ V. Reprinted with permission from Ref. [39]. Copyright 2024, Springer Nature.

lastingly prevents molecular structure from oxidation damage but also passivates the latent electron traps to stabilize electron transport. This antioxidant strategy demonstrated excellent uniformity and batch-to-batch reproducibility in large-area OFET arrays. Complementary inverters fabricated using this approach likewise exhibited higher gain and superior environmental stability. This study presents a way to overcome the long-standing stability problem of n-type OSCs and devices.

SUMMARY AND OUTLOOKS

With the rapid advancement of organic electronic devices, researchers have recognized that trace oxygen molecules engage in intricate physicochemical interactions with organic semiconductor materials, having profound impact on charge transport properties and long-term operational stability of OSCs and their electronics. The deep understanding and modulation strategies of these interactions between trace oxygen and organic molecular systems will provide new insights for charge transport and powerful practical methodologies for molecular doping technology. This perspective summarizes research on the mechanisms of oxygen doping in OSCs and recently related modulation strategies. The role of oxygen in OSCs can be multiple involving carrier trapping, photo-oxidation and acceptor doping, in light of the material systems, environment and interactions. The ingenious utilization of trace oxygen through delicate modulation strategies can significantly enhance the performance and stability of OSCs and devices.

In the future, the oxygen doping technology would be more generalized to apply into diverse optoelectronic materials, including conducting polymers, luminescent molecules, as well as emerging material systems such as perovskites and two-dimensional (2D) materials. Such technology would enable their optimized application in photovoltaics, OLEDs, and other optoelectronic devices, provided that targeted modulation strategies are carefully designed based on material-specific electronic structures and doping mechanisms. The stability problems of doping interfaces would be emergent challenges due to the diffusion tendency of small oxygen molecules.

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Conflict of interest The authors declare that they have no conflict of interest.

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有机半导体中的痕量氧掺杂: 机理解析与精准调控

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摘要 有机半导体是一类新型半导体材料，在可穿戴电子、柔性显示、生物传感等领域具有广阔的应用前景. 有机半导体的聚集态结构由弱范德华力支配，其性能极易受到外源杂质等非本征因素的影响. 近年来，有机半导体中杂质来源及其影响机制的研究取得了显著进展. 氧是有机半导体中最常见的外来杂质，长期被视为电荷陷阱，导致迁移率下降并影响器件稳定性. 最近的研究报道了氧掺杂在痕量水平上产生截然相反的作用，即痕量氧掺杂能够显著提高有机电子器件的性能和稳定性. 在未来，深入理解痕量氧与有机分子体系相互作用机制并发展分子水平的氧掺杂调控策略将为有机固体电荷输运研究提供新见解和强有力的应用技术. 本文阐明了有机半导体中痕量氧掺杂现象的基本原理，并探讨了最先进的氧掺杂调控技术及其对器件性能和稳定性的影响. 最后，提出了氧元素掺杂工程的发展框架，同时概述了其在新兴材料与器件领域中应用的新挑战.

