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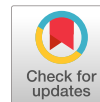
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Multivalent oxide-cluster ion doping for functionalizing semicrystalline polymer semiconductors

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Molecular doping has enabled control of electronic properties in semiconducting polymers for studies of charge transport and device applications. However, conventional dopant anions are mostly organic monovalent species whose roles are largely limited to stable charge compensation. Here, we introduce polyoxometalates as multivalent oxide-cluster dopant ions into semicrystalline polymer semiconductors. In particular, films doped with size-compatible divalent $[\text{W}_6\text{O}_{19}]^{2-}$ retain lamellar order, exhibit conductivity above 200 S cm^{-1} , and show a Hall response, indicating partially coherent carrier transport. Compared with inert-anion-doped films, $[\text{W}_6\text{O}_{19}]^{2-}$ -doped films show enhanced anodic response in the oxygen-evolution region, demonstrating functional multivalent-ion doping for electronic and electrocatalytic polymer semiconductor films. © 2026 The Author(s). Published on behalf of The Japan Society of Applied Physics by IOP Publishing Ltd

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Molecular doping, which introduces molecular dopants into semiconducting polymer films through redox reactions, is a key strategy for controlling their electronic properties.¹⁾ Solution-processable polymer semiconductors provide large-area and mechanically compliant thin films for electronic and optoelectronic devices, including photovoltaic cells,^{2,3)} organic thermoelectrics,^{4,5)} and circuit elements such as transistors and diodes.^{6–9)} In these applications, molecular doping can control carrier density, tune energy-level alignment, reduce contact resistance, and enable high electrical conductivity in polymer semiconductor films.

Recent advances in ion-exchange and related doping strategies have expanded the accessible range of dopant ions in semiconducting polymers.^{10–14)} In ion-exchange doping, redox reactions first generate charged polymer chains with exchangeable counterions, which are subsequently replaced by dopant ions supplied from solution. Dopant-ion design has been shown to affect doped-state stability, energetic disorder, microstructure, charge transport, thermoelectric performance, and the formation of highly crystalline doped thin films.^{15–17)} These studies indicate that dopant ions are not merely passive charge compensators; their size, charge density, and spatial arrangement can strongly influence the structure-property relationships of doped polymer semiconductors. Recent studies have shown that organic dopant dianions or dianionic counterions can be incorporated into polymer semiconductors, offering a route to dense charge compensation with fewer counterions.^{18,19)} Such multivalent dopant species can also strongly modulate the electronic states of doped polymers, including the promotion of bipolaron formation.²⁰⁾ However, dianion-dominated regimes have mainly been demonstrated at relatively low dopant fractions, with conductivities of only

a few S cm^{-1} . This leaves room for new multivalent dopant ions that combine dense charge compensation, structural compatibility, and additional molecular functionality.

Polyoxometalates (POMs) are promising candidates for functional dopant ions because they are multivalent oxide-cluster ions with tunable redox and catalytic properties.^{21–27)} A Keggin-type POM, phosphomolybdic acid, has been used for solution-based p-doping of semiconducting polymers.^{3,28)} If incorporated as dopant ions in ordered polymer semiconductor films, POMs could provide dense multivalent charge compensation while also introducing oxide-cluster-based interfacial functionality. A central challenge is that POMs are much larger and more highly charged than conventional organic monoanions. Their incorporation into semicrystalline polymer semiconductors would disrupt lamellar packing and deteriorate carrier transport if the dopant size is incompatible with the polymer nanostructure.²⁹⁾ Therefore, size-compatible dopant design is essential for introducing multivalent oxide-cluster ions into ordered polymer films without sacrificing semicrystalline order.

Here, we demonstrate the incorporation of POMs into semicrystalline poly(2,5-bis(3-tetradecylthiophen-2-yl)thieno[3,2-*b*]thiophene) (PBTtT) films by anion-exchange doping. Unlike larger Keggin-type POMs previously used for polymer doping, the smaller Lindqvist-type $[\text{W}_6\text{O}_{19}]^{2-}$ anion is compatible with the PBTtT lamellar nanostructure, allowing divalent oxide-cluster ions to be incorporated while preserving the ordered film structure. The resulting POM-doped PBTtT films exhibit electrical conductivity above 200 S cm^{-1} and show a Hall response, indicating partially coherent carrier transport in the organic-inorganic hybrid semiconductor film. As a demonstration of interfacial electrochemical functionality, the POM-doped



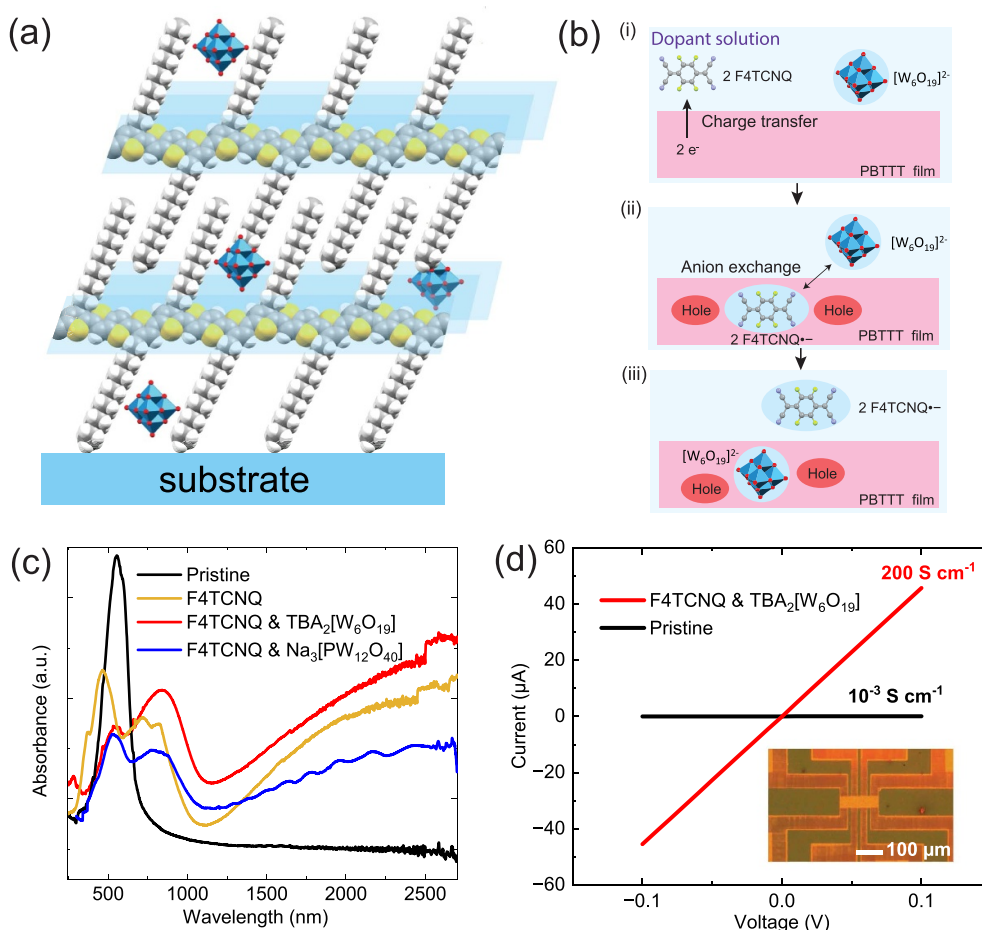


Fig. 1. Anion-exchange doping using POMs. (a) Illustration of $[\text{W}_6\text{O}_{19}]^{2-}$ -doped PBTtT. (b) Schematic of anion exchange from $\text{F4TCNQ}^{\bullet-}$ to $[\text{W}_6\text{O}_{19}]^{2-}$. (c) Optical absorbance spectra of PBTtT films before and after the treatment with dopant solutions. (d) Conductivity of pristine and $\text{F4TCNQ}/\text{TBA}_2[\text{W}_6\text{O}_{19}]$ -treated PBTtT films.

films also show an enhanced anodic response in the oxygen-evolution region compared with PBTtT films doped with an inert molecular anion. These results highlight POM doping as a versatile strategy for functionalizing semicrystalline polymer semiconductors with multivalent oxide-cluster ions, opening opportunities to explore electronic transport and interfacial electrochemical functionality in ordered hybrid films.

The progress of anion exchange doping was confirmed by UV–Vis–near-IR (NIR) absorption spectroscopy and conductivity measurements of PBTtT thin films (Figs. 1(c) and 1(d)). Spin-coated PBTtT films were immersed in a doping solution containing $\text{TBA}_2[\text{W}_6\text{O}_{19}]$ (TBA = tetra-*n*-butylammonium) and 2,3,5,6-tetracyanoquinodimethane (F4TCNQ). In the pristine PBTtT film, an absorption peak attributed to the π – π^* transition appeared around 550 nm.³⁰⁾ After immersion in the F4TCNQ solution, the intensity of this peak decreased, and new features emerged around 800 nm and in the NIR region, consistent with p-type doping of PBTtT.^{10, 31, 32)} The peaks at 730 and 830 nm are attributed to the $\text{F4TCNQ}^{\bullet-}$. When doping solutions containing F4TCNQ together with either $\text{TBA}_2[\text{W}_6\text{O}_{19}]$ as the Lindqvist-type POM source or $\text{Na}_3[\text{PW}_{12}\text{O}_{40}]$ as the Keggin-type POM source were used, the peaks associated with $\text{F4TCNQ}^{\bullet-}$ became negligible, while the spectral features of doped PBTtT remained. These results

provide strong evidence for the successful anion-exchange doping of PBTtT with $[\text{W}_6\text{O}_{19}]^{2-}$ and $[\text{PW}_{12}\text{O}_{40}]^{3-}$. For $[\text{PW}_{12}\text{O}_{40}]^{3-}$, the Na^+ salt was specifically employed because TBA salts did not enable efficient anion exchange under these conditions. The anion-exchange efficiency for various POMs is discussed in the Supplementary Information (Fig. S1). Conductivity measurements further support this conclusion. The conductivity of the PBTtT thin film with thickness of 50 nm, increased from approximately $10^{-3} \text{ S cm}^{-1}$ to 200 S cm^{-1} through this doping process (Fig. 1(d)).

The introduced dopant anion was identified by X-ray photoelectron spectroscopy (XPS, Fig. 2(a)). While the pristine PBTtT thin film exhibited C 1s and S 2p peaks, O 1s and W 4f peaks were observed after treatment with the $\text{F4TCNQ}/\text{TBA}_2[\text{W}_6\text{O}_{19}]$ solution. Under the employed doping condition, the F 1s signal disappeared completely (Fig. S2), confirming nearly quantitative replacement of $\text{F4TCNQ}^{\bullet-}$ -derived anions by the introduced POM species.

Quantitative XPS analysis (Figs. 2(b)–2(d) and Table I) gave an incorporation ratio of one $[\text{W}_6\text{O}_{19}]^{2-}$ per 4.1 PBTtT monomer units from the C/W atomic ratio. Because $[\text{W}_6\text{O}_{19}]^{2-}$ is dianionic, this composition corresponds to approximately one hole per two PBTtT monomer units. This doping level is reasonable compared with F4TCNQ-doped PBTtT, where one hole is generated per approximately three monomer units.³¹⁾ Anion exchange can shift the doping

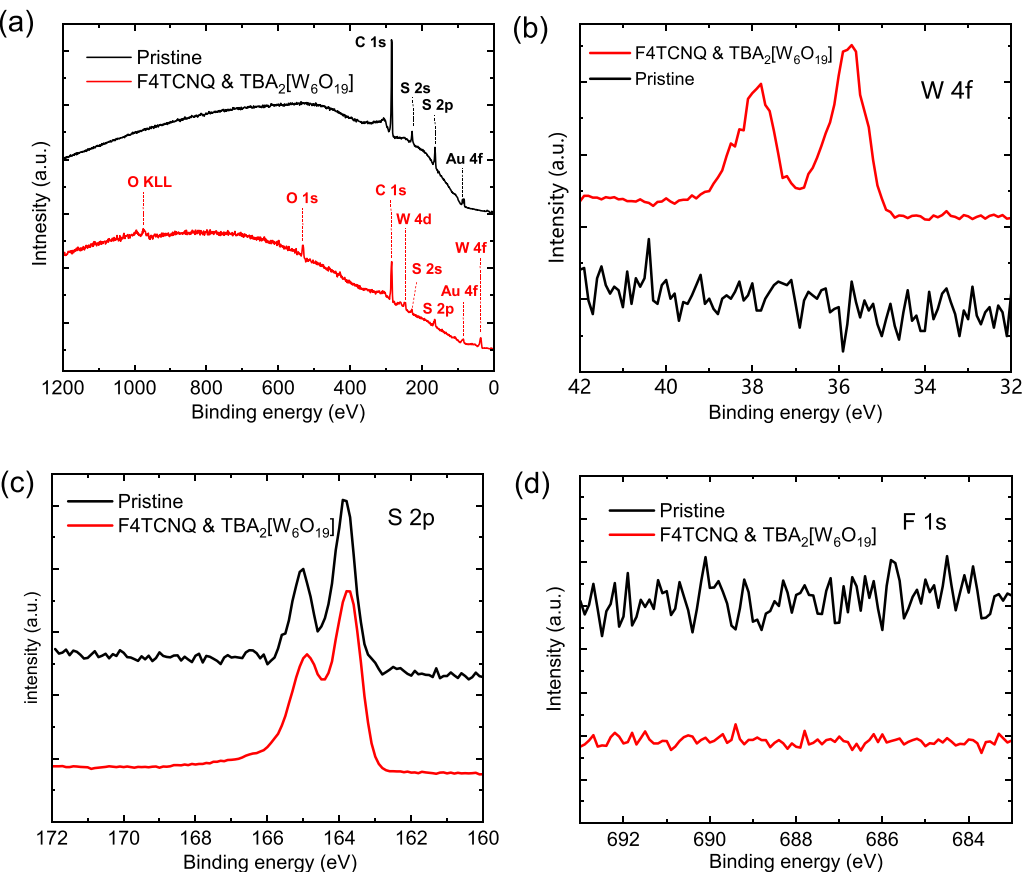


Fig. 2. XPS analysis of PBTBT thin films. (a) Wide-scan XPS spectra and narrow-scan spectra in the (b) W 4f, (c) S 2p, and (d) F 1s regions for pristine and F4TCNQ/TBA₂W₆O₁₉-treated PBTBT thin films.

Table I. XPS elements analysis of atomic concentration [%].

	C	S	W	O	F	N
Pristine	92.4	7.2	—	0.4	—	—
TBA ₂ W ₆ O ₁₉ -treated	80.9	5.6	2.8	10.8	—	—

equilibrium toward higher oxidation states compared with F4TCNQ doping,¹⁰⁾ consistent with the higher doping level observed in our XPS and UV–Vis–NIR spectra. The W 4f peak positions indicate that the incorporated tungsten species remain predominantly in the W(VI) state, consistent with incorporation of [W₆O₁₉]^{2−} without significant reduction or decomposition.

Grazing-incidence wide-angle X-ray scattering (GIWAXS) measurements showed that PBTBT retains an edge-on orientation after doping with [W₆O₁₉]^{2−} (Figs. 3(a)–3(c)). The structural parameters extracted from the line profiles are summarized in Table II. Upon [W₆O₁₉]^{2−} doping, the lamellar spacing increased, whereas the out-of-plane FWHM was nearly unchanged (Fig. 3(e)), indicating that the lamellar order was preserved. The in-plane peak shifted to higher q_{xy} and slightly narrowed (Fig. 3(d)), suggesting a reduced π -stacking distance and improved in-plane ordering.^{10, 31, 33)} These results indicate that [W₆O₁₉]^{2−} anions are mainly incorporated into the alkyl side-chain regions without disrupting the conjugated backbone packing. In contrast, doping with the larger [PW₁₂O₄₀]^{3−} anion caused substantial peak broadening in both directions, indicating significant structural disorder.

Carriers in semicrystalline PBTBT thin films doped with [W₆O₁₉]^{2−} exhibit band-like transport characteristics, as evidenced by Hall effect measurements. At 200 K, the Hall voltage (V_H) showed a linear dependence on the applied magnetic field (Fig. 4(a)), confirming the presence of delocalized carriers. From linear fitting of the Hall voltage as a function of magnetic field (Fig. 4(b)), the carrier density and Hall mobility at different temperatures were extracted. However, the Hall mobility was only 0.26 cm² V^{−1} s^{−1} (Fig. 4(c)), lower than that of F4TCNQ^{•−} (1.8 cm² V^{−1} s^{−1})³¹⁾ or monoanion-doped (2.4 cm² V^{−1} s^{−1}) PBTBT.¹⁰⁾ This reduced Hall mobility may arise from hopping carriers that partially suppress the Hall voltage,³⁴⁾ likely because of electrostatic potential fluctuations induced by the dianionic dopant ions. Note that, in such a mixed transport regime, the Hall carrier density is overestimated. Consistent with this interpretation, the overall conductivity follows a variable range hopping (VRH) transport (Fig. 4(d)). The temperature-dependent conductivity showed good agreement with the VRH model (Fig. S3), suggesting a hopping contribution exists. Together with the Hall response described above, this result supports a mixed transport picture in which band-like and hopping transport components coexist in the [W₆O₁₉]^{2−}-doped PBTBT film.

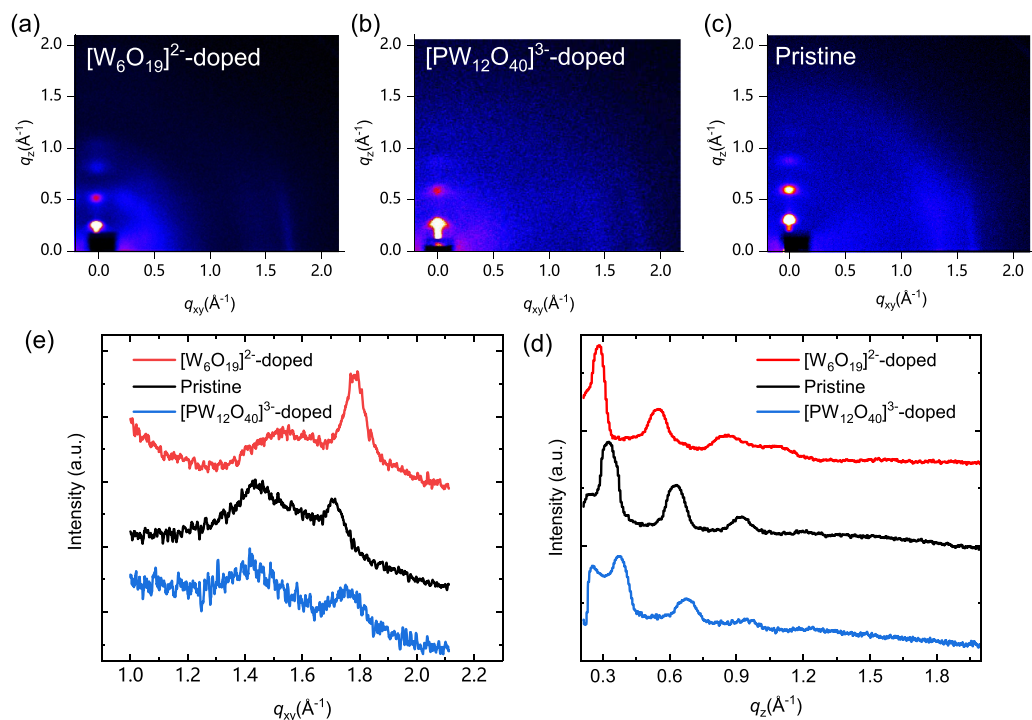


Fig. 3. GIWAXS analysis of PBTBT. 2D GIWAXS patterns of (a) $[W_6O_{19}]^{2-}$ -doped, (b) $[PW_{12}O_{40}]^{3-}$ -doped, and (c) pristine PBTBT thin films. (d) In-plane (q_{xy}) and (e) out-of-plane (q_z) GIWAXS line profiles of pristine and doped PBTBT thin films.

Table II. Structural parameters extracted from GIWAXS analysis of pristine and POM-doped PBTBT films.

	Lamellar distance (Å)	Out-of-plane FWHM (Å ⁻¹)	π -stacking distance (Å)	In-plane FWHM (Å ⁻¹)
Pristine	21.4	0.011	3.65	0.095
$[W_6O_{19}]^{2-}$ -doped	24.9	0.012	3.52	0.070
$[PW_{12}O_{40}]^{3-}$ -doped	20.9	0.133	3.59	1.751

As an additional functionality, we evaluated the anodic response of the POM-doped polymer films in the oxygen-evolution-reaction (OER) potential region. Measurements were performed using a standard three-electrode setup in aqueous H_2SO_4 solution (pH 2). PBTBT films were drop-cast on glassy carbon (GC) electrodes and doped with POM or bis(trifluoromethanesulfonyl)imide (TFSI[−]), a conventional inert counteranion that can yield highly conducting PBTBT films.¹⁰⁾ Current densities were normalized to the geometric area of the GC electrode.

Linear sweep voltammetry (LSV) curves show that $[W_6O_{19}]^{2-}$ -doped PBTBT exhibited a higher anodic current density than $[PW_{12}O_{40}]^{3-}$ -doped and TFSI[−]-doped PBTBT in the OER potential region (Fig. 5(a)). This comparison indicates that the enhanced anodic response is not simply explained by electronic conductivity. The $[W_6O_{19}]^{2-}$ -doped electrode also showed a smaller apparent Tafel slope than the TFSI[−]-doped and GC electrodes (Fig. 5(b)), suggesting more favorable interfacial charge-transfer behavior.

Controlled-potential electrolysis at 1.8 V vs. RHE further showed that the $[W_6O_{19}]^{2-}$ -doped PBTBT maintained a higher current than the TFSI[−]-doped film over the measurement period (Fig. 5(c)), suggesting a more stable electrochemical interface under oxidative conditions. Electrochemical impedance spectroscopy (EIS) also showed that the $[W_6O_{19}]^{2-}$ -doped PBTBT electrode had a lower

charge-transfer resistance ($R_{ct} = 345 \text{ } \Omega \text{ cm}^2$) than the $[PW_{12}O_{40}]^{3-}$ -doped electrode ($721 \text{ } \Omega \text{ cm}^2$) (Fig. 5(d)). The larger impedance of the $[PW_{12}O_{40}]^{3-}$ -doped film is consistent with its greater structural disorder observed by GIWAXS, which may hinder interfacial charge transfer. R_{ct} was substantially larger than the high-frequency intercept of less than $30 \text{ } \Omega \text{ cm}^2$, which represents the combined series resistance arising from the electrolyte, electrode contacts, and electronic conduction through the polymer film. This indicates that the impedance response under the present conditions is dominated by the interfacial charge-transfer process rather than by electronic transport through the polymer film. The electrochemically active surface area (ECSA) estimation is described in the Supplementary Information (Fig. S4). The estimated ECSA is consistent with only a limited, electrolyte-accessible region near the surface of the polymer film contributing directly to the electrochemical reaction. Thus, the observed electrochemical functionality is governed primarily by dopant ions incorporated in the near-surface region, rather than by electrochemical processes occurring throughout the full film thickness, which would require diffusion of water and other reactant species into the hydrophobic film interior. The enhanced anodic response is consistent with previous studies of tungsten-oxide-based surfaces,^{35, 36)} although W-based oxides and non-functionalized W/Mo/V POMs are not among the most active standalone water-oxidation

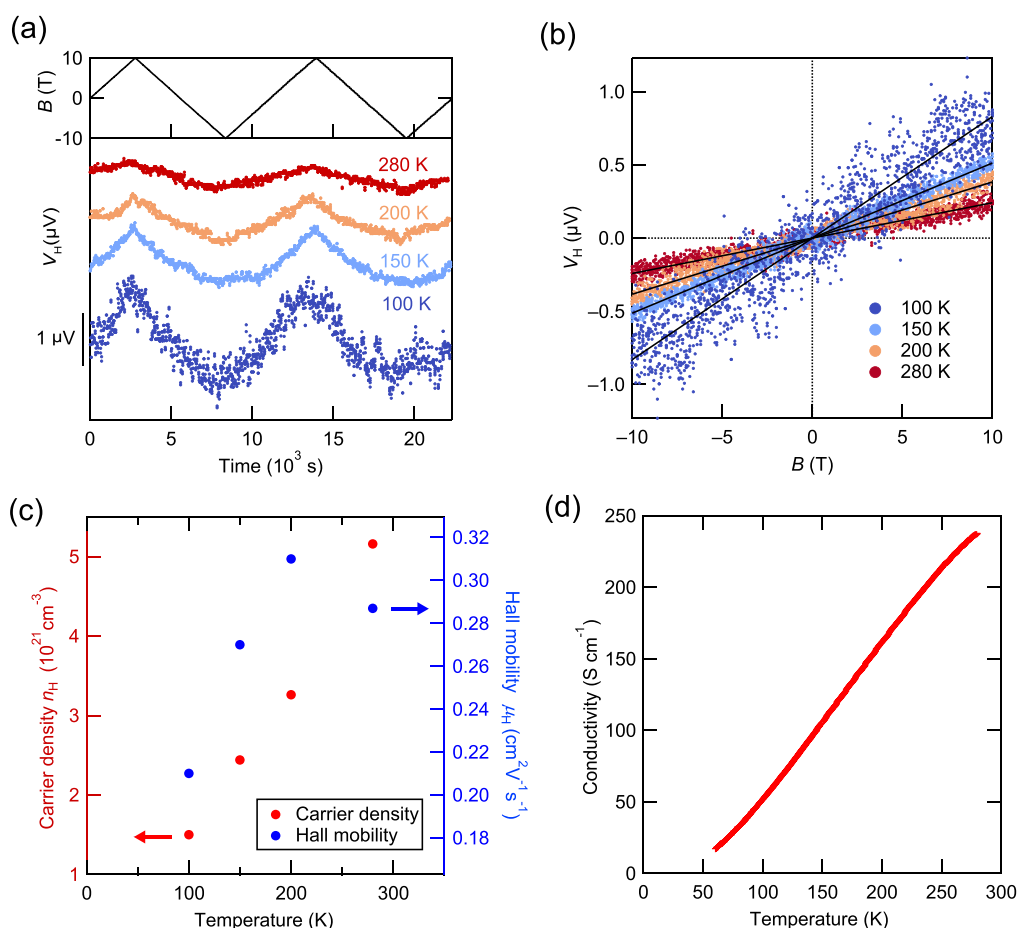


Fig. 4. Hall measurements of a $[\text{W}_6\text{O}_{19}]^{2-}$ -doped PBTTT thin film. (a), (b) Hall voltage measured under magnetic fields at different temperatures. (c) Extracted carrier density and Hall mobility. (d) Temperature-dependent electrical conductivity.

catalysts.³⁷⁾ Further exploration of POM structures and doping processes may therefore enable systematic control of both transport and interfacial functionality in semicrystalline polymer semiconductor films.

We have demonstrated the incorporation of POMs into semicrystalline PBTTT films by anion-exchange doping. $[\text{W}_6\text{O}_{19}]^{2-}$ was compatible with the PBTTT lamellar nanostructure and could be incorporated while preserving the ordered film structure, yielding conducting organic–inorganic hybrid semiconductor films with a conductivity of 200 S cm $^{-1}$. Hall-effect and temperature-dependent conductivity measurements reveal partially coherent carrier transport coex-

isting with hopping-like conduction in the divalent-anion-doped polymer semiconductor. The POM-doped films also show an enhanced anodic response in the oxygen-evolution potential region compared with inert-anion-doped PBTTT, indicating interfacial electrochemical functionality beyond stable charge compensation. These results highlight POM doping as a versatile strategy for functionalizing semicrystalline polymer semiconductors with multivalent oxide-cluster ions. Because the charge, size, shape, and composition of POMs are tunable, such tunability may open opportunities to explore charge transport and interfacial electrochemical functionality in semicrystalline thin films.

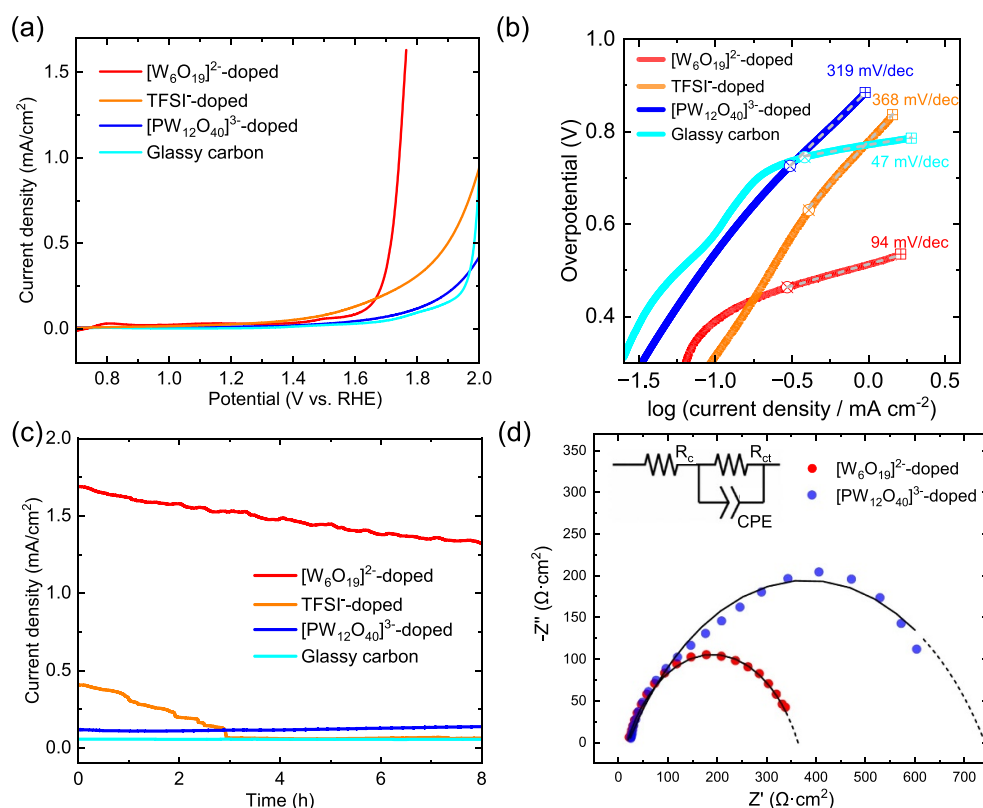


Fig. 5. Electrochemical response of POM-doped PBTTT films in the oxygen-evolution potential region. (a) Linear sweeping voltammetry (LSV) at a scan rate of 10 mV s^{-1} and (b) Tafel plots of doped PBTTT and glassy carbon electrodes. (c) Controlled-potential bulk electrolysis in pH 2 electrolyte at 1.8 V vs. RHE. (d) Nyquist plots of POM-doped PBTTT electrodes recorded in pH 2 electrolyte at 1.8 V vs. RHE over a frequency range from 100 kHz to 10 Hz. Inset: equivalent circuit used for fitting, where R_c is the contact resistance, R_{ct} is the charge-transfer resistance, and CPE denotes the constant-phase element.

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