Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Large electric piezoresistance of the flexible molecular semiconductive crystal $Q(TCNQ)_2$ during bending

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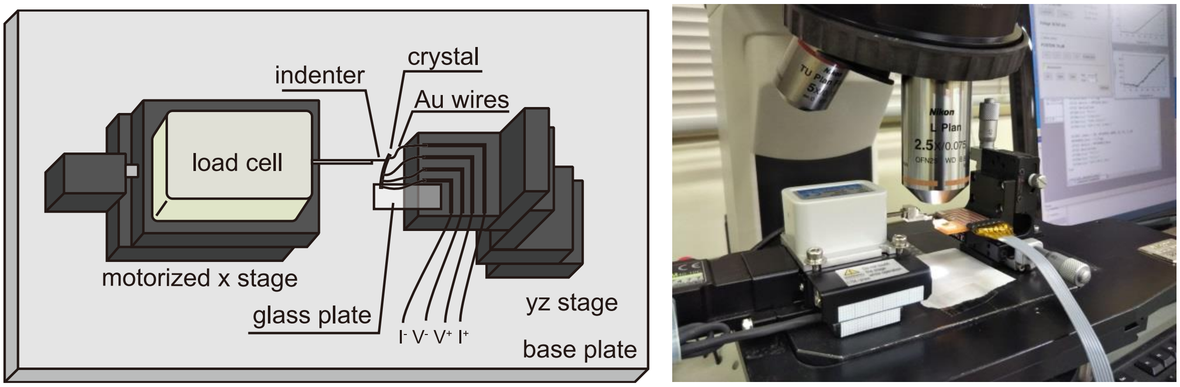
Contents

Experimental Methods.

Electrical resistivity measurements during the stress-strain test were performed using a homemade apparatus equipped with a micro-load cell (LTS-50GA, Kyowa Dengyo) mounted on a motorized optical stage (TAMM40-10C, Sigma-Koki). One side of the crystal was attached to the glass plate using cyanoacrylate, while the other side was pressed by an indenter (silicon AFM tip, NSC35/AlBS, MikroMasch) attached to the load cell. The motorized stage was stepped 10 μm at 5-second intervals (0.12 mm/min). An AC voltage (2.0 V_{p-p}, 10 Hz) was applied to the input terminals of the load cell, and the output voltage was acquired using a lock-in amplifier (LI5640, NF Corporation). The electrical resistance of the bent crystal was measured using a four-probe method with a voltmeter (34401, Hewlett-Packard) and current source (3245A, Hewlett-Packard). Electric connections were made using gold wires (10 μm φ) and gold paste (No. 8560, Tokuriki). During the stress-strain test, a DC current of 1 mA was applied to the crystal, and the generated voltage was recorded. Electronic instruments were controlled using the software Igor Pro 7.0 (Wavemetrics).



Schematic and photograph of the measurement apparatus.

Calculation Methods for the stress-strain curves.

The configurations for the three-point loading and cantiveler tests are shown below. In the three-point test using the standard method (ISO 178:2019 and ASTM D0790-10), the flexural stress σ_f and flexural strain ε_f were calculated using the following equations:

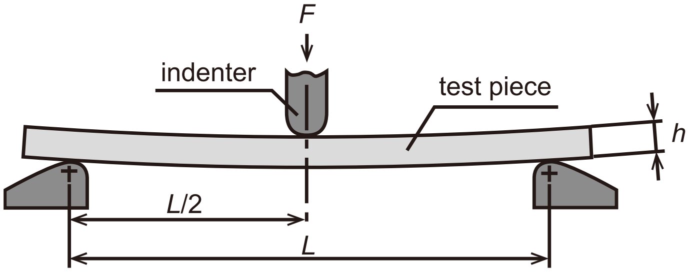
$$\sigma_\mathrm{f} = \frac{3FL}{2bh^2} \qquad , \qquad \varepsilon_\mathrm{f} = \frac{6sh}{L^2}$$

where *F, b,* and *s* denote the applied force, width of the test piece, *and* deflection, respectively.

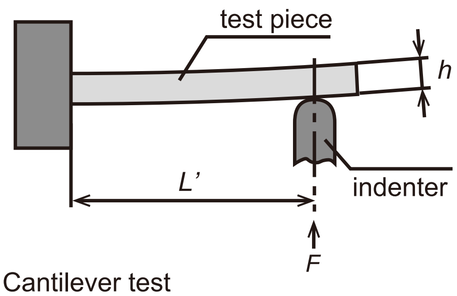
As shown in the diagram, the cantilever test had a configuration of half that of the three-point loading test. By substituting *L* into the above equations with $L = 2L'$, the following equations are obtained:

$$\sigma_\mathrm{f} = \frac{6FL'}{2bh^2} \qquad , \qquad \varepsilon_\mathrm{f} = \frac{3sh}{2L'^2}$$

In this study, the stress-strain curve was calculated using the above equations.



Three-point loading test



Cantilever test

Configurations for the three-point loading and cantilever tests.

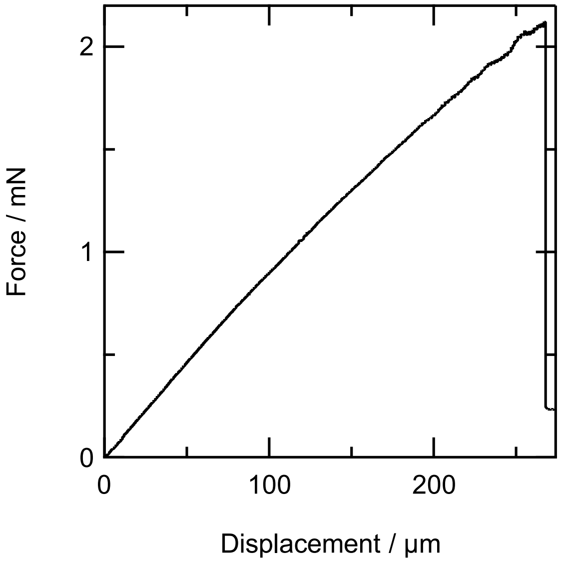


Figure S1. Raw data for the bending test of a Q(TCNQ)$_2$ crystal along *c* axis.

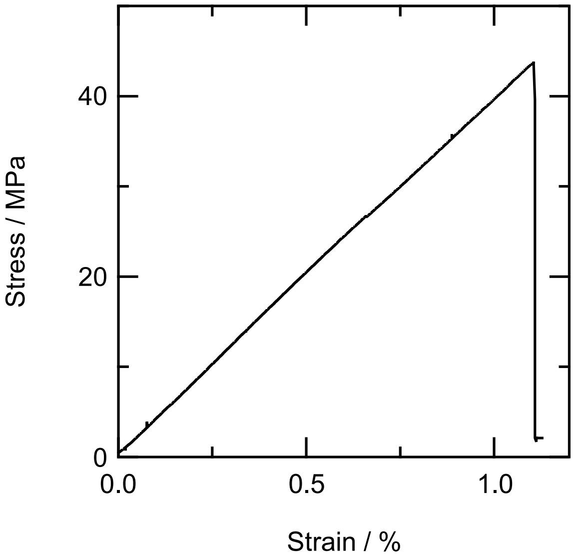


Figure S2. A stress-strain curve during the electronic resistance measurement.

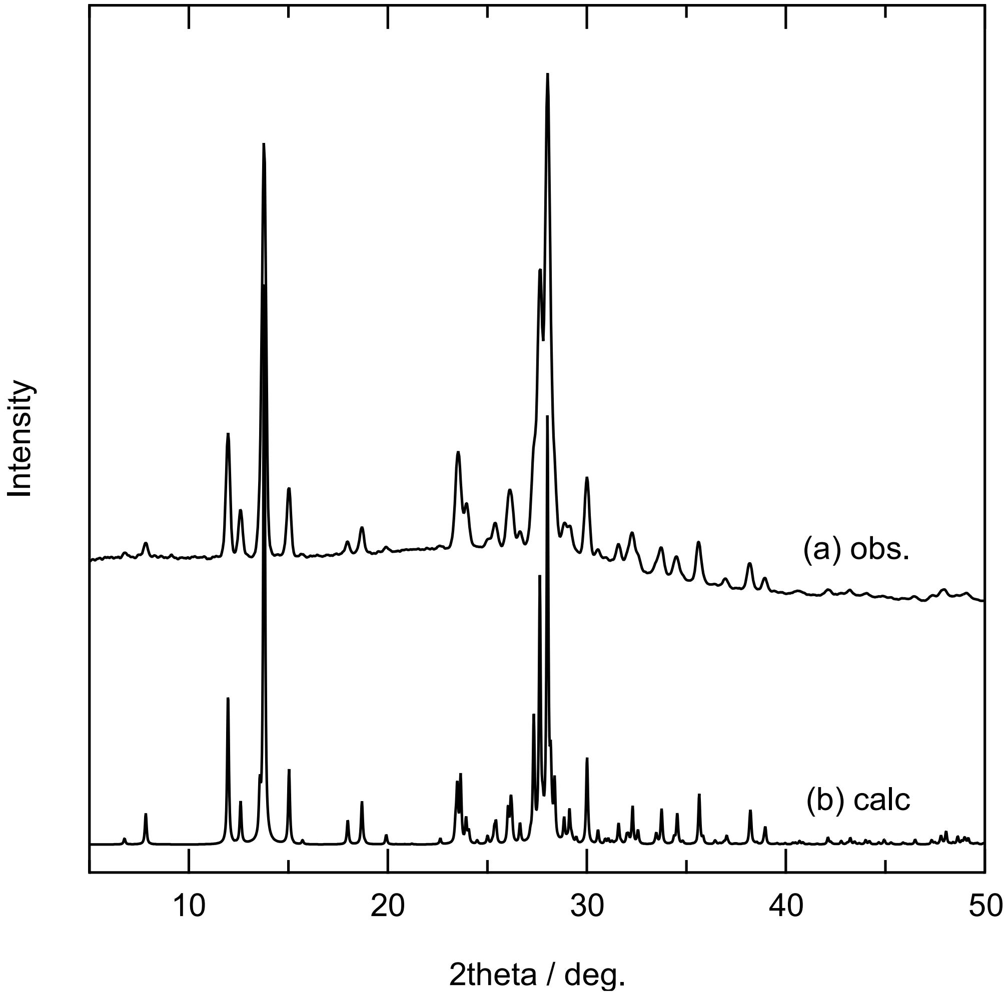


Figure S3. Powder XRD data for Q(TCNQ)$_2$. (a) Observed for the granulated crystals at 300 K. (b) Calculated for the literature data in ref. 12.