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## Thermal Narrowing of the Electronic Bandwidths in Organic Molecular Semiconductors: Impact of the Crystal Thermal Expansion

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### Abstract

We report on electronic-structure calculations for the pentacene and rubrene crystals, based on experimental crystal geometries measured at different temperatures. The results are in very good agreement with angle-resolved photoelectron spectroscopy data that indicate that the widths of the valence and conduction bands in both materials become narrower at higher temperatures. Our findings strongly suggest that the thermal bandwidth narrowing in the pentacene and rubrene crystals is primarily caused by the thermal expansion of the lattice rather than by a renormalization of the transfer integrals induced by a polaron effect. The effect of thermal expansion on the charge-transport properties is also discussed.

### Keywords

**KeyWords Plus:** CHARGE-TRANSPORT; SINGLE-CRYSTALS; NAPHTHALENE; PENTACENE; MOTION

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