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Modifying the Optoelectronic Properties of Rubrene by Strain[1]
SAHAR SHARIFZADEH, Department of Electrical and Computer Engineering, Boston University, ASHWIN RAMASUBRAMANIAM, Department of Mechanical Industrial Engineering, University of Massachusetts Amherst — Rubrene crystals are promising organic electronic and optoelectronic materials due to their high charge carrier mobility. Recent studies have shown that the electronic properties of rubrene films can be tuned by substrate-induced strain, suggesting a new route towards the design of more efficient devices. Here, we present a first-principles density functional theory and many-body perturbation theory analysis of strain-induced changes to the mechanical, electronic, and optical properties of rubrene crystals. With an applied strain that is consistent with experiment, we predict changes of hole motilities in excellent agreement with electrical conductivity measurements. Furthermore, we predict that the optical absorption and nature of low-energy excitons within the crystal can be tuned by an applied strain as low as 1%.

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