

Review of: "Correlating exciton coherence length, localization, and its optical lineshape"

Daniel Vanmaekelbergh¹

¹ Utrecht University

Potential competing interests: No potential competing interests to declare.

This work uses a classic analytical model to understand the line-shape and width of the emission spectrum for molecular excitons in a disordered polymer-type medium that structurally responds to an exciton. The line shape and width is related to a competition between self-trapping by a structural reorganization (assumed to occur also at “zero temperature”) and thermal fluctuations. The (de) localization of the exciton wavefunction is important in this competition. The authors aim to present a model in which the exciton line-shape and width reflects the structural and dynamic properties of the polymer medium.

In my opinion the results are new and important enough to warrant publication. Below, I present some suggestions to make the work better readable for a more general audience.

COM1: In the abstract and through the text, the authors use the concept of exciton line shape, but never show or address the functional form of the line shape (gaussian?) in their work. Besides this, the result of the model is an additional width, a line shape is not discussed as an outcome of the model, in contrast to the statement in the abstract. I believe that additional information should be given on this issue.

COM2: related to this, Fig. 1 presents an important result; the additional homogeneous width due to thermal fluctuations for a range of assumed exciton reorganization energies. Please explain: additional to what?

COM3: Moreover, the manuscript starts with the concept of “self-trapping” of the exciton in an elastic (polymeric) medium – fair enough – but can this self-trapping also occur when the lattice is at 0 Kelvin? In other words, is the static self-trapped exciton a physical reality?

COM4: The relation between exciton self-trapping and reorganization energy should be explained more explicitly.