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Origin of non-Gaussian site energy disorder in molecular aggregates

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Abstract

Gaussian site energy disorder is an ad hoc concept usually implemented in simulations of excitation dynamics in molecular systems. In this letter we suggest a mechanism which may cause correlated static energy disorder in a broad range of molecular systems. Our approach leads to non-Gaussian site energy distribution, which strongly affects statistical properties of exciton wavefunctions and consequently changes material functional characteristics.

Keywords: excitons, gaussian disorder, molecular aggregates

1. Introduction

Technologically relevant molecular materials at ambient temperature are usually understood as microscopically unordered systems. Their equilibrated