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Optimized Configuration Interaction Method for Electronic Excitations in Nanostructures[1] CLAUDIA TROPAREVSKY, Oak Ridge National Laboratory and National Renewable Energy Laboratory, ALBERTO FRANCESCHETTI, National Renewable Energy Laboratory — The Configuration Interaction (CI) method has been widely used to calculate electronic excitations in semiconductor nanostructures. The main drawbacks of this method are its slow convergence with the number of configurations and the difficulty to select a-priori the most relevant configurations. Here we report a new approach for the selection of the CI basis set: For a given number N_C of configurations, we use heuristic search methods to find the set of N_C configurations that minimizes the excited-state energy of the nanostructure. We demonstrate this method for single excitons and biexcitons in CdSe quantum dots. We show that the best configurations not only are different from what one would expect based on the single-particle energy ladder, but also, they often do not correspond to the configurations that have the largest contribution to the full CI wave function. We also show that a few (less than 100) optimized configurations provide excitation energies with accuracy comparable to much larger (10,000 or more) non-optimized configuration basis sets.

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