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Optical Absorption Spectra Calculated Using Linear-Scaling ...

The development of linear-scaling density functional theory (LS-DFT) has made ab initio calculations on systems containing thousands of atoms possible.

Calculating optical absorption spectra for large systems ...

PHYSICAL REVIEW B 84, 165131 (2011) Calculating optical absorption spectra for large systems using linear-scaling density functional theory Laura E. Ratcliff,^{*} Nicholas D. M. Hine, and Peter D. Haynes

Calculation of Optical Absorption Spectra using a ...
 ABSTRACT CALCULATION OF OPTICAL ABSORPTION SPECTRA USING A SUPERVISED NEURAL NETWORK Conrad W. Rosenbrock
 Department of Physics and Astronomy Bachelor of Science

Optical Absorption Spectra and Excitons of Dye-Substrate ...

Here, we calculate the optical absorption spectra and spatial distribution of bright excitons in the visible region for a prototypical DSSC, catechol on rutile TiO₂(110), as a function of coverage and deprotonation of the OH anchoring groups. This is accomplished by solving the Bethe-Salpeter equation (BSE) based on hybrid range-separated exchange and correlation functional (HSE06) density

Self-interaction-corrected time-dependent density ...

Self-interaction-corrected time-dependent density-functional-theory calculations of x-ray-absorption spectra
 Guangde Tu, Zilvinas Rinkevicius, Olav Vahtras, and Hans gren^{*}

Optical-absorption coefficient measurements in solids and ...

Optical-absorption coefficient measurements in solids and liquids using correlation photoacoustic spectroscopy
 optical-absorption coefficients in the solid and liquid states. 2. Instrumentation and materials A schematic diagram of the experimental apparatus is shown in Fig. 1. Light sources used for optical excitation of the samples were a 1-mW He-Ne laser, or the light from a 1000-W Xe
 Analysis and assignment of the optical absorption ...

Some vibrational and electronic properties of the CuCl₂ molecule are analyzed in order to characterize the electronic states and assign the bands seen on the optical absorption spectra.

Theory and calculations of X-ray spectra: XAS, XES, XRS ...

These findings highlight that, given the overall agreement between experimental and calculated spectra, the Cr₂AIC electronic structure is accurately predicted using density functional theory.

Predicting Raman Spectra Using Density Functional Theory - OSA

Tips for preparing a search: Keep it simple - don't use too many different parameters. Separate search groups with parentheses and Booleans. Note the Boolean sign must be in upper-case.

Calculating Optical Absorption Spectra of Thin ...

The ability of our approach to predict absorption spectra is demonstrated using the example of polycrystalline films of 3,4,9,10-perylenetetracarboxylic diimide (PTCDD).

Introduction Thin films of conjugated organic molecules are essential building blocks in organic and hybrid optoelectronics.

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