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ELECTRONIC BAND STRUCTURE FROM FINITE CLUSTER CALCULATIONS



Anna Pomogaeva
Electronic band structure
from finite cluster
calculations
Basics, Methodology, Applications

Condition: New. Publisher/Verlag: VDM Verlag Dr. Müller | Basics, Methodology, Applications | Nowadays computation progress can provide very accurate predictions for relatively large molecular systems. For extended systems, if there exists periodicity, one can take into account the periodic boundary conditions. However, such calculations still have a lot of difficulties especially in treating non-periodic perturbations even for one dimension systems. In the present work an alternative method is proposed which extracts an accurate band structure of polymers from oligomer calculations....

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