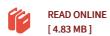




Calculations on nonlinear optical properties for large systems The elongation method SpringerBriefs in Molecular Science SpringerBriefs in . Properties of Atoms, Molecules, and Clusters

By -

Springer. Paperback. Condition: New. 98 pages. For design purposes one needs to relate the structure of proposed materials to their NLO (nonlinear optical) and other properties, which is a situation where theoretical approaches can be very helpful in providing suggestions for candidate systems that subsequently can be synthesized and studied experimentally. This brief describes the quantum-mechanical treatment of the response to one or more external oscillating electric fields for molecular and macroscopic, crystalline systems. To calculate NLO properties of large systems, a linear scaling generalized elongation method for the efficient and accurate calculation is introduced. The reader should be aware that this treatment is particularly feasible for complicated three-dimensional andor delocalized systems that are intractable when applied to conventional or other linear scaling methods. This item ships from multiple locations. Your book may arrive from Roseburg, OR, La Vergne, TN. Paperback.



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