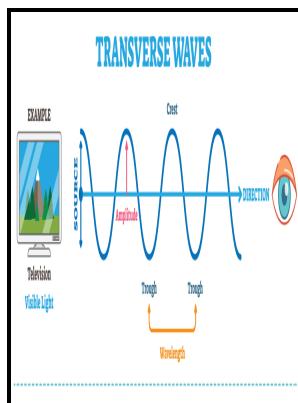


# Application of wave mechanical methods to the study of molecular properties.

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Muller, Jan Florián, Arieh Warshel. The MD model is an effective tool for designers to optimize the IPL sintering process.

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The Journal of Physical Chemistry A 2007, 111 38 , 9573-9585.

## A Quantum Mechanical and Molecular Mechanical Method Based on CM1A Charges: Applications to Solvent Effects on Organic Equilibria and Reactions

Real-Time Time-Dependent Electronic Structure Theory. Gamache, Impact-induced Glass-Transition in Elastomeric Coatings, Appl. Dillon, Development and Parameterization of a Time-invariant equilibrium Material Model for Segmented Elastomeric Polyureas, J.

## Quantum Mechanical Method

Because subsequent particles start their vibration one after the other with a slight time delay, the vibrational motion travels with a finite velocity  $c$  known as the wave velocity.

## Molecular Properties from Combined QM/MM Methods. 2. Chemical Shifts in Large Molecules

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