

Israel Journal of Chemistry



Official Journal of the Israel Chemical Society

Computational Molecular Biophysics

Guest Editors: Yaakov Levy, Jeffrey Skolnick

8–9/2014

www.ijc.wiley-vch.de

$H\psi = E\psi$

$-\frac{\partial U}{\partial r} = m \frac{d^2 r}{dt^2}$

$\sum_{\text{angles}} K_{\theta} (\theta - \theta_0)^2$

$\sum \epsilon_{ij} \left(\frac{\sigma_{ij}}{r} \right)^{12}$

$\sum \left\{ \epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r} \right)^{12} - 2 \left(\frac{\sigma_{ij}}{r} \right)^6 \right] \right\}$

$\sum_{\text{bonds}} K_b (b - b_0)^2$

$\sum_{\text{dihedrals}} K_{\varphi} [1 - \cos(n\varphi - \varphi_0)]$

Volume 54

WILEY-VCH

Cover Picture

This special volume focuses on Computational molecular biophysics in honor of the 2013 Nobel Prize in Chemistry awarded to Karplus (right), Levitt (middle), and Warshel (left). In a series of seminal contributions, the three laureates provided novel approaches to study complex chemical systems. The cover shows the fundamental energy terms used in many transferrable force-fields to calculate the structure of a variety of biomolecules. Force-fields are still widely used, both in atomistic or coarse-grained forms, to decipher the conformational landscape (represented by the white curve) of proteins and their folding mechanism. The cover also illustrates the achievement of the Nobel laureates to study the action of an enzyme (the cover highlights Lysozyme that breaks polysaccharides into smaller fragments) by carefully integrating quantum and classical calculations. See the Guest Editorial on page 1039.

