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## 國立陽明大學生醫光電研究所 🖲

Institute of Biophotonics National Yang Ming University



學術專題演講 瑞士聯邦理工學院物理化學實驗室 Wilfred F. van Gunsteren 教授

## Thirty years of (Bio)molecular simulation: How far have we come?

Prof. Wilfred F. van Gunsteren



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Computation based on molecular models is playing an increasingly important role in biology, biological chemistry, and biophysics. Since only a very limited number of properties of biomolecular systems is actually accessible to measurement by experimental means, computer simulation can complement experiment by providing not only averages, but also distributions and time series of any definable – observable or non-observable – quantity, for example conformational distributions or interactions between parts of molecular systems....

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