Faculty of Computer Science & Department of Chemistry Seminar

Informatics: synthesis of experiment and calculation

By

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Refreshments will be served at 3:20 p.m.

How can computers help chemists? It is now possible to handle chemical information effectively using computers, but there is still some justifiable reluctance to use computational methods in some experimental research groups. What useful information can be gained from computational studies? I will describe examples of experiment and calculation working together to gain a better understanding of molecular structure and reactivity.