PLENARY 3

THEORETICAL MODELLING OF FLUOROCARBONS

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New developments in theory and software coupled with the availability of supercomputers now make it possible to reliably calculate many important properties of fluorinated materials, including molecular structures, dynamic behaviour, infrared vibrational modes, and free energies of formation. This presentation will illustrate how numerical simulations based on molecular orbital theory can be used to compliment experiment in prediction the properties and behaviour of fluorocarbons ranging from small chlorofluorocarbons to high molecular weight fluoropolymers. Examples where theory both augments experiment, as in the visualization of vibrational motion in fluoropolymer chains, and corrects experiment, as in the revision of heats of formation for $CFCl_3$ and CF_2Cl_2, will be presented. Theoretical studies of chain conformations that relate to the helicity of polytetrafluoroethylene, $\{CF_2CF_2\}_n$, the piezoelectric behaviour of polyvinylidene fluoride, $\{CH_2CF_2\}_n$, and the electronic properties of polyfluoroacetylenes, $\{CF{=}CF\}_n$ and $\{CH{=}CF\}_n$, also will be described. The challenges and prospects of using the computer to ultimately predict bulk physical properties and to design new materials will be addressed.