CFEL SCIENCE

SEMINAR

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Optical centrifuge simulations of polyatomic molecules

The preparation of molecules in highly excited rotational states has opened up interesting avenues of research in chemical dynamics. An efficient technique for creating such states is an optical centrifuge [1]. Using non-resonant laser fields, molecules are trapped and then forced to follow the rotating polarization of a centrifuge field. By gradually increasing the field's angular frequency, molecules can be accelerated into extremely high rotational states. In certain instances even up to dissociation.

In this talk, I will discuss robust, fully quantum mechanical simulations of a polyatomic molecule in an optical centrifuge. The approach taken is applicable for any small molecule but is computationally demanding and requires several stages of calculations. As an illustrative example I will present results on phosphine (PH_3). This is an interesting molecule because rotational energy level clusters appear at high rotational excitation [2]. The resultant “cluster states” are known to be chiral [3], leading to the concept of dynamic chirality. An optical centrifuge is perhaps the most effective way to populate these states and explore their properties.

[1] J. Karczemarek, J. Wright, P. Corkum and M. Ivanov, Phys. Rev. Lett. 82, 3420, (1999).
[2] S. N. Yurchenko, W. Thiel, S. Patchkovskii and P. Jensen, Phys. Chem. Chem. Phys. 7, 573, (2005).
[3] P. R. Bunker and P. Jensen, J. Mol. Spectrosc. 228, 640, (2004).

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