

Postdoc position

Dynamics of molecule formation on ices: thermal or UV-induced?

Applications (deadline January 20 2009) are invited for a 22 months postdoc position for theoretical research on the dynamics of chemical reactions on ice surfaces at the Leiden Institute of Chemistry and Leiden Observatory of Leiden University, The Netherlands. The research will be carried out in the framework of a collaboration between the Theoretical Chemistry group (Prof. G.J. Kroes) and the Astrochemistry group (Prof. E.F. van Dishoeck), with funding from the Netherlands Organization for Scientific Research NWO on a TOP-project "The role of excited electronic and vibrational states in chemical reactions on surfaces". A description of the research is given below.

Applications should include a curriculum vitae, a brief statement of research experience, and arrange for at least two letters of reference to be sent to the address below. Selection of candidates will start on January 20 2009 and will continue until the position is filled. The position is open to all nationalities with a PhD in chemistry, physics or astronomy. The starting date for the position is flexible up to fall 2009. Please send applications to:

Prof. dr. E.F. van Dishoeck
Leiden Observatory
P.O. Box 9513
2300 RA Leiden
The Netherlands

FAX: +31-71-5275819
e-mail submission: jobs@strw.leidenuniv.nl
e-mail inquiries: ewine@strw.leidenuniv.nl

See

<http://www.theorchem.leidenuniv.nl/>
<http://www.strw.leidenuniv.nl/~ewine/>

Project description

In dense interstellar clouds where new stars and planets are formed, small dust particles (consisting of ~0.1 micron silicates) are covered by ice mantles consisting of H₂O, CO, CO₂, CH₄ and other species, at a temperature of about 10 K. Recent observations show that larger molecules such as H₂CO, CH₃OH, and HCOOH may be present as well. These molecules can either form by thermal hydrogenation and oxidation reactions of smaller molecules such as CO, or by photon-induced processes.

In this project, the above mentioned reactions are studied by performing molecular dynamics simulations to "make" particles of amorphous ice in the computer. Next, reactions on the surface of such

particles will be modelled using quantum transition state theory. In addition, classical trajectory calculations will be performed to obtain mechanistic insights into the most important pathways, and to visualize these reactions. Subsequently, the effects of UV photons, which can dissociate the H₂O ice to form energetic OH and H, will be considered. Reactions of energetic OH with CO is thought to be a principle route to form CO₂. The central goal of the project is to determine which chemical reactions can occur on interstellar ices, and to determine the dominant reaction mechanisms: thermal or UV. If time permits, photodesorption processes of simple ices will be modelled as well. Complementary laboratory experiments on these reactions are being carried at the Sackler Laboratory at Leiden Observatory.

Term of appointment: 22 months

Required: PhD in Chemistry, Physics, or Astronomy, with an interest in molecular dynamics. Experience with numerical methods and computer programming is a prerequisite.

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