

The Warwick Lecture in Theoretical Chemistry

Hosted by the Measurement and Modelling Cluster



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4.00 pm, Physics Lecture Theatre, Science Concourse. ALL WELCOMED

‘Exploring Hydrated Electrons in Non-Conventional and Conventional Ways: *From Alkali Metal Explosions to Non-Explosive Ways*’

A dangerous but among school kids all-time favorite experiment demonstrating an explosive chemical reaction is throwing a piece of sodium in water. Every high school chemistry teacher knows that the explosion is due to release of electrons from the metal to water accompanied by formation of steam and molecular hydrogen, which can ignite during this exoergic process. The very same gases should, however, separate the reacting metal and water and thus quench the reaction. How come the explosion occurs anyway? Using ultrafast cameras and ab initio as well as force field molecular dynamics simulations we have discovered a hitherto unknown primary mechanism of the explosive behavior of alkali metals in water. Namely, after migration of electrons from the metal to water the former acquires a huge positive charge. Thanks to mutual repulsion of these charges the metal undergoes a Coulomb explosion accompanied by ejection of metal spikes into water. This enables effective mixing of reactants, which is a necessary condition for the explosion. As an extra bonus, we also show how blue solvated electrons formed during this reaction can be observed with a naked eye despite their sub-millisecond lifetime in water.