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Simulating Laser-Induced Dynamics in Next Generation Photo-Acid Materials for EUVL (JCLV3)

Background

Photolithography is a top-down approach to computer chip manufacture[1], which embeds patterns onto computer chips. It uses a light source to drive structural changes in molecules. Extreme ultra-violet lithography (EUVL) uses 13.5 nm photons generated by a tin plasma light source[1,2]. EUV lithography has been demonstrated to successfully produce sub 7 nm nodes and has been used in the manufacture of Apple's new M1 chips. Photoacid generators (PAGs) are light sensitive materials that when exposed to specific wavelengths of light, convert into a strong acid with high efficiency[2,3] used to speed up or chemically amplify resists. One of the key performance factors with regards to PAGs is the dose of light required for effective photo-initiation[2]. Sensitivity is thus a key metric to consider for high volume manufacturing[1,2], as good sensitivity not only reduces the exposure time, meaning a higher volume output, but it also means that there is a higher likelihood of the pattern being formed. Thus, it is of key interest to deduce the key photochemical pathways that these materials undergo, which can then be used to develop new, more sensitive materials.

This project is part of a SFI funded research programme on the structure and dynamics of molecules that could be relevant to EUVL resists. It will focus on a variety of computational techniques that will be used to elucidate laser induced dynamics in these materials. Using quantum chemical software packages, such as ORCA 5.03, the steady-state electronic structure will be determined, via the calculation of UV-Vis and emission spectra[4]. The excited state electron density will be computed and the decomposition process of the photoacid generator will be modelled in order to identify the key electronic pathways that lead to the formation of the acid. Following the successful completion of the latter work, surface hopping methods will be employed to qualitatively track nonadiabatic dynamics[5] in the PAG systems on a variety of timescales (from femtoseconds to nanoseconds). These results will then be compared to complementary experimental results obtained in DCU.

You will work on the computational aspects of the work on local computing platforms and possibly on ICHEC (www.ichec.ie). You will work with Postdoc Lazaros Varvarezos, assisted by PhD students Ross McGarry (Chemical Sciences) and Stephen Durkan (Physical Sciences).

References

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