Coulomb Crystals – Towards a greater understanding of chemical bonding

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Since Paul Traps were developed in the late eighties, they have provided a way of studying chemical species and their reactions in a very dense and extremely cold environment. When trapped, ionised species form an ordered state called a Coulomb Crystal, which can be made to fluoresce with an appropriately tuned laser, and the light is then captured by a microscope.

This allows chemists to work with a cleaner signal when studying how reactions progress, as the species should be almost all in the ground state, and collisions should be frequent enough to be experimentally practical.

Due to its lack of an activation energy, one of the simplest reactions is between an ionised species and a neutral species, the theory of which has remained essentially unchanged since 1905. Interpreting the fluorescence images of the crystals is demanding and it can take up to an hour of trained experimenter's time to find the number of species. To streamline this process, BlueBear is being used to simulate the data and train a machine learning model that can analyse an image in seconds.