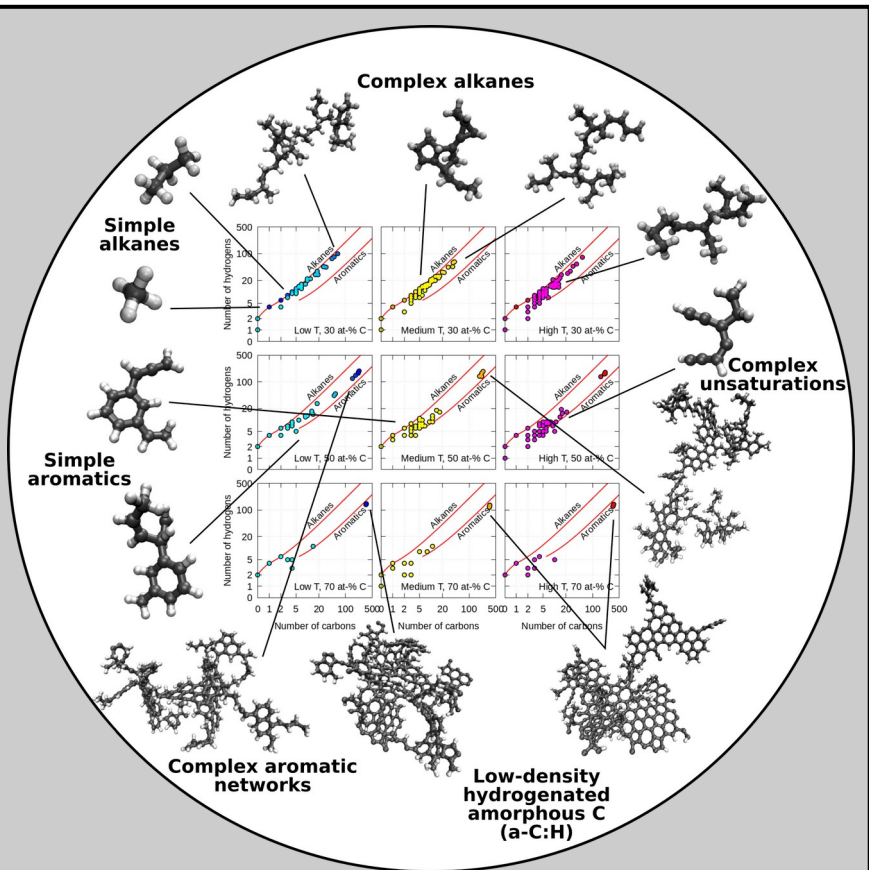


**Project title:** *Next-generation interatomic potentials to simulate new cellulose-based materials (2003146 NEXTCELL)*

Our developed CH potential has “learned” how to handle almost any chemical reaction that takes place between carbon and hydrogen, producing very complex molecules and networks



**INFO BOX**

- **What:** We have used iterative training to learn the potential energy surface describing the different ways in which C and H can bind to one another to form stable structures of arbitrary complexity. This force field is fully reactive (in addition to stable structures, it can handle the chemical reactions leading to them).
- **Why:** Having a general-purpose and accurate force field for the CH system lets us understand hydrogenated carbon-based materials and is a first step along the road to obtain a fully reactive CHO potential, which will allow us to handle complex organic chemistry.
- **Who:** Mikhail Kuklin (main contributor) and Miguel Caro (PI).