

Recipes For Any Occasion. Computational Chemistry and the Desktop Computer

Johannes Lenhard (Bielefeld)

In general terms, this talk is about how mathematization and technology are intertwined. I will address this topic in a more particular way, namely I am interested in computational modeling, and even more particular: I'll talk about so-called density functional theory (dft), a widely used method that is located in the intersection of computational physics and chemistry. In fact, dft seems to enjoy a phenomenal success. I'll argue that this success mirrors a boost for computational methods that began in the late 1980s. It is based on an explorative and iterative mode of computational modeling that came in use when computational power became easily available on small computers.