ACCURATE AB INITIO MOLECULAR CALCULATIONS FOR ULTRACOLD PHYSICS EXPERIMENTS

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Cold and ultracold systems attract researchers' attention because the world's quantum nature clearly manifests under such conditions. Research into such systems provides new insight into the quantum theory of matter and matter-light interactions. Ultracold atoms and molecules offer numerous exciting research prospects ranging from quantum-controlled chemical reactions and quantum simulations to precision spectroscopic measurements probing the fundamental laws of nature.

I will present how *ab initio* molecular electronic structure and multichannel scattering calculations can propose, guide, and explain ultracold quantum physics experiments. I will discuss the capabilities and limits of present methods applied to systems based on alkali-metal and alkaline-earth-metal atoms. I will start with our theoretical predictions of the scattering lengths for ultracold collisions without any adjustment to experimental data, which were possible by including high-level-correlation, relativistic, QED, and adiabatic corrections[1]. I will conclude with our theoretical explanations of quantum resonances measured in ultracold atom-ion[2],[3] and atom-molecule[4] collisions, where the quantum regime of cold collisions and their quantum control with an external magnetic field have been recently reached for the first time.

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