**TEMPLATE FOR ABSTRACTS**

**Going big and complex**

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The use of novel methods from scientific computing and advances made in the field of computational chemistry and physics allow us to study increasingly large systems and to address more complex molecular properties.[1,2] These developments allow computational methods to be applied to ever-larger systems, increasingly enabling us to study the full system investigated in experiment and to study ever more sophisticated nonlinear experiments involving the interaction of strong electric and magnetic fields with molecules and solids.

In this talk, I will outline some of the advances made in our group in the study of nonlinear and higher-order molecular properties by building on novel techniques developed in the field of scientific computing, such as recursive programming[3] and automatic differentiation.[4] Applications of these methods will be highlighted for anharmonic corrections to vibrational properties[5] and in the study of two- and multiphoton absorption properties.[6,7]

I will also outline how we can develop numerically efficient methods for the study of relativistic effects in molecules and solids, solving the Dirac-Kohn-Sham equation for individual molecules and for systems with periodic boundary conditions applied. Examples of the study of spin-orbit effects in 2-dimensional materials will be given, with calculations involving more than 900 000 Gaussian basis functions in four-component relativistic calculations.[8] I will show that relativistic calculations on solids now can be performed with only small additional costs compared to similar non-relativistic calculations.

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[8] Kadek, M.; Repisky, M.; and Ruud, K., *in preparation.*