

BERNOULLIS TAFELRUNDE

GRADUATE STUDENT SEMINAR

Thursday, 17 December, 12:15-13:00
Seminarraum 00.003, Spiegelgasse 1

MONICA BUGEANU

Universität Basel

Calculating the energy of molecules.

**A computational introduction to chemistry and wavelet
boundary element methods.**

ABSTRACT

In this talk I will try to explain the concept of the polarizable continuum model and how boundary element methods can be used in combination with it to obtain the energy of molecules in solvent. I will present the practical aspects of building a solver and the difficulties that we have encountered.