

Seminarreihe Materialforschung & Physik

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**“Gas Phase Structures –  
Experiment and Theory”**

**Mittwoch, 17. Mai 2017,  
17:00 s.t., SR I,  
Jakob-Haringer-Strasse 2a, JAK2AOG1.33**

The determination of molecular structures by electron diffraction is described. An example is discussed in which this method determines not only molecular structures but also a chemical process. The combination of the experimental method with quantum chemical calculations is of great advantage for the experiment and is a good test for the reliability of theoretical methods. Several examples are given, where some quantum chemical calculations (ab initio or density functional methods) do not agree with experimental structures or conformational properties.