

**Einladung
zum
Physikalischen Kolloquium
Montag, 10.07.2017
16:15 Uhr in N24/H13**

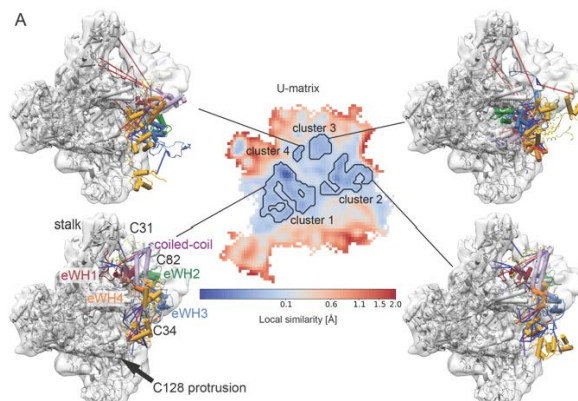


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Modeling macromolecular complexes from conflicting and ambiguous data

The multiple sources of structural data used in hybrid structure determination of macromolecular complexes poses new challenges: data may be much more sparse than in high resolution methods; data sets from heterogeneous sources may be of highly different and unknown quality and may be mutually inconsistent; data sets from different sources may have very different information content; and data are in general averaged over large ensembles and long measurement times. In addition, structural knowledge of different components of the complex may be available to rather different degrees. Hence, with hybrid methods, the treatment of structure determination as an inference problem is even more important than in high resolution structure determination. For NMR structure determination, we introduced an approach that treats structure determination rigorously as an inference problem, based on Bayesian probability theory, which we called Inferential Structure Determination and implemented in the program ISD (Rieping2005). I will briefly introduce the underlying concepts. I will then discuss more recent work on the development of this framework for the determination of structures from various data sources, and for the determination of larger systems (Ferber2016).

Rieping W, Habeck M, Nilges M. Inferential structure determination. *Science*. 2005 Jul 8;309(5732):303-6
Ferber M, Kosinski J, Ori A, Rashid UJ, Moreno-Morcillo M, Simon B, Bouvier G, Batista PR, Müller CW, Beck M, Nilges M. Automated structure modeling of large protein assemblies using crosslinks as distance restraints. *Nat Methods*. 2016 Jun;13(6):515-20



Ab 16.00 Uhr Kaffee, Tee und Kekse vor dem Hörsaal H13

Organisation: Prof. Dr. F. Jelezko, Tel. 23750

Host: Prof. Dr. J. Michaelis, Tel. 23050 off.: 23051