

## Séminaire de Chimie Théorique

Salle réunion groupe THEO 3ème Est, Bat. A12  
Mardi 24 Octobre 2017 à 11:00h

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### Cheap and near exact calculations with large active spaces : New applications

I will present new features and applications of the semi-stochastic heat-bath configuration interaction (SHCI) algorithm[1], which allows near-exact calculations with large active spaces of systems of interest in biological processes and energy conversion and storage. In particular, the new CASSCF with large active space feature[2] and applications to relativistic effects[3] will be demonstrated.

[1] Sharma, Holmes, Jeanmairet, Alavi, Umrigar JCTC (2017)

[2] Smith, Mussard, Holmes, Sharma JCTC (2017)

[3] Mussard, Sharma JCTC (2017)