

### 1. Aim & motivation:

The aim of the requested STSM is to explore current possibilities and future challenges in the field of an equal quantum mechanical treatment of the electrons and the atomic nuclei.

The imminent goal of the proposed STSM is the preparation of background material (draft for a review paper) for the Task Force 3 Meeting ( <http://www.compchem.hu/molim-tf3/> ) of MOLIM.

As to the longer-term objectives, we have in mind various research topics in this field which could grow out from a longer term collaboration of the host (Patrick Cassam-Chenaï) and the visitor (Edit Matyus). We would like to dedicate time for the discussion of these topics during the planned visit.

### 2. Proposed contribution to the scientific objectives of the Action:

The Actions's Memorandum of Understanding mentions the "handling of coupled electron and nuclear motions" among its goals. The primary focus of our theoretical developments is high-resolution spectroscopy,

so our contributions are directly connected with the activity of working group (WG) 1, but it is also related to WG2.

### 3. Techniques:

We wish to discuss in detail and identify future challenges for the non-Born-Oppenheimer methods recently developed by the participants (host and visitor):

- P. Cassam-Chenaï, B. Suo, W. Liu - PRA 92, 012502 (2015) & TCA 136, 52 (2017).

- E. Mátyus and M. Reiher, JCP 137, 024104 (2012)& E. Mátyus, PCA 117, 7195 (2013).

### 4. Planning

The visit will start with the review and compilation of all material already available for the TF3 Meeting and review paper. Next, we will prepare discussion topics for the Meeting which could help to identify the key elements of the review paper. During this work, we will also identify particular open challenges in the field (e.g., molecular structure conundrum) and define the necessary steps to solve them in a longer-term collaborative project of the host and the visitor.