UNIVERSITÀ
DEGLI STUDI DI TRIESTE
Dipartimento di Scienze Chimiche e Farmaceutiche
Associate Prof. Sonia Coriani, Ph.D.
E-mail: coriani@units.it; Tel. +390405583947 (direct)

To the kind attention of

Professor Attila G. Császár
COST MC Chair (MOLIM)
Eötvös University, Budapest, Hungary

and

Prof. Nadja Doslic,
Ruđer Boškovic Institute,
Zagreb, Croatia

Trieste, 30/11/2016

LETTER OF SUPPORT FOR STSM

Dear Professor Császár,

It is my pleasure to invite Dr. Aurora Ponzi to visit the Theoretical Chemistry group at the University of Trieste from January 9 to February 9, 2017, within the COST MOLIM scheme, to work on the project "Coupled Cluster studies of photoionization observables". Dr. Ponzi is currently postdoctoral researcher in the group of dr. sc. Nađa Došlić at the Ruđer Boškovic Institute, Zagreb, Croatia. As outlined in the research plan – Dr. Ponzi will work on the integration of our currently developed Coupled Cluster approach to compute Dyson orbitals for ground and excited states, with a multi-centric DFT B-spline code for the electronic continuum. The methodology developed will subsequently be used to simulate UPS and XPS observables in molecular systems where electron correlation is expected to play an important role, and include the evaluation of nuclear dynamics effects. We expect this STSM to further strengthen the long-term collaboration between Prof. Došlić's group and the Theoretical Chemistry group in Trieste, and to result in a number of peer reviewed papers of high quality, as well as open source program modules, e.g. in the Dalton program (www.daltonprogram.org).

During her stay in Trieste, Dr. Ponzi will have access to an office space equipped with a desktop computer and full internet access, plus access to large-scale computing resources through my personal CPU grant at the CINECA supercomputer centre in Italy.

Sincerely Yours,

Sonia Coriani