



## Charter for EMMC working group on *Electronic models*

### Background and role of the WG

Within the European Materials Modelling Council (EMMC), working groups (WGs) focusing on selected topics have been formed to help increase the impact of materials modelling on the European economy and society. This will be achieved by promoting modelling quality development and the efficient use and organisation of both existing and future resources in the field of materials modelling (i.e. models, methods, software, and modelling infrastructure). The EMMC should also advise the European Commission in matters relating to modelling and provide input for future EC strategies, visions and plans.

The electronic structure community is the largest community of modellers in Europe, both in terms of number of actors and HPC usage. Information from electronic structure calculations is required in a range of situations where information at the detail of electronic models, or at the accuracy of high-level QM calculations is needed. This could concern the information about the most likely route of a chemical reaction, the consequences of defects in a material, the relative stability of crystal polymorphs for use in pharmaceutical industry, or the design of more powerful magnetic materials.

In addition to such examples where materials properties and processes depend explicitly on the behaviour of the electrons (the electronic wavefunction) there are a number of other circumstances where calculations using electronic models, i.e. quantum-mechanical (QM) calculations, are needed. One example is QM calculations for the generation of ab initio-derived quantities that can directly be used as parameters in more coarse-grained or continuum models, typically when experimental parameters are not available. Another example is the generation of data that can serve as a training-set for the parametrization of more coarse-grained interaction model (e.g.  $e \Rightarrow a$ ), or the reverse procedure, when some interesting phenomena or structure "observed" using an atomistic-model simulation needs to be scrutinized at the level of detail given by an electronic model.

The report "*Preparation of a LEIT Materials Modelling Policy*" from the 27 February 2014 LEIT meeting in Brussels highlighted that, among end-users and manufacturers, the most frequently mentioned modelling issues in need of attention were "Reliability", "Validation & References" and "Integration of models and codes". The *Electronic models* WG focuses on the first two of these. There are a number of phenomena that are not yet possible to describe accurately with today's electronic models for materials calculations. Examples are dispersion interactions in the DFT models, highly correlated materials, ... XX [more examples to be added]. *This WG will focus on improving the reliability and applicability of electronic structure models for industrially relevant contexts.*

## Scope of the WG

The scope of the WG encompasses two main tracks of modelling efforts: on the one hand, the improved and wider exploitation of *existing* models, and on the other, the development of *new or improved*, more accurate (yet computationally feasible) electronic structure models of industrial relevance.

Both wave-function based and DFT-based models belong here, as do the various approaches to explore the potential energy landscape, methods for advanced property calculations, not least in the context of experimentally measurable quantities, where experiment provides the data needed for validation and the QM calculations provide the missing details to assist the experimental approach. XX KH: Not exactly part of the model itself- but certainly crucial to make the methods applicable to realistic industrial problems.XX

Molecules constitute an intrinsic part of materials modelling in at least two different contexts: molecular materials and Some very important applications of materials involve the interaction between materials surfaces and molecules.

In summary: The WG aims to promote the targeted development of electronic models to improve their reliability and applicability in industrially relevant contexts.

## Objectives

- To push the boundaries of QM-based materials modelling closer to realistic applications.
- To develop an interaction with other established organisations of the electronic structure community, such as CECAM and Psi-k.
- To foster interactions with the a/m/c communities and with the Coupling and Linking od Models WG as well as with the Validation WG.
- To act as a sounding board and participate in European consultation initiatives.

## Goals

- Define the main challenges associated with the objective.
- Establish short-term and long-term working approaches towards the objectives.
- Establish a core team and develop a (representative) network of engaged actors in the Coupling and Linking WG.

## Desired outcome

To fulfil the objectives.

## Timeline

- October 2014 Invitation to Nov meeting of active contributors by EC
- Working Group Meeting on 5/6 November in Brussels
- Completion of a first Road Map by end Q1 2015
- Continuously: Expanding database to reach a representative social network with active core team

### **Current team members**

Kersti Hermansson, Uppsala University

Roy Chantrell, The University of York

Pietro Asinari, Politecnico di Torino, yes?

Nicola Marzari, EPFL