

To whom it may concern

Institut Lumière Matière

UMR5306 CNRS
Université Claude Bernard Lyon 1
Domaine Scientifique de La Doua
Bâtiment Kastler, 10 rue Ada Byron
69622 Villeurbanne CEDEX, FRANCE

<http://llm.univ-lyon1.fr>

T +33 (0)4 72 43 29 93

FAX +33 (0)4 72 43 11 30

E-mail contact.ilm@univ-lyon1.fr

M. Paul Ceria did his stage of M2 in 2012 under my direction for a period of around five months. The topic of his project was the theoretical determination of metastable phases of carbon under pressure using state-of-the-art structural prediction methods. The only input for these methods is the atomic composition of the solid (and the pressure). Studies of this kind had been performed within density functional theory (DFT) and relatively small unit cells (up to 8 or 16 atoms). The main objective of this project was to go beyond this number, and use cell sizes of up to 48 atoms. This implied having to switch from DFT to a more “economical” (but less precise) theory, namely tight-binding to evaluate enthalpies and forces.

During this period, M. Ceria gained a good working knowledge of the minima hopping method (the global structural prediction method we currently use). He also understood well how to use the codes necessary for this stage and the rather complex workflow to perform his simulations. He found several novel structures representing hexagonal or cubic diamond with defect planes and lines, that were later characterized using DFT by other collaborators. This results have just been published in Phys. Rev. B. [“Carbon structures and defect-planes in diamond at high pressure”, S. Botti, M. Amsler, J.A. Flores-Livas, P. Ceria, S. Goedecker, M.A.L. Marques, Phys. Rev. B **88**, 014102 (2013)]. Unfortunately, health problems during the period of the writing of the report and especially during the “soutenance”, did not allow M. Ceria to have a grade that he desired and that he certainly deserved.

I believe that M. Ceria's most important quality is his motivation and his perseverance. He is a very motivated young man that shows a lot of enthusiasm for his work. I have therefore no doubt that he is capable of pursuing a PhD.

With my best regards,



(Miguel Alexandre Lopes Marques)