



Alan McGaughey
Associate Professor
Department of Mechanical Engineering
Carnegie Mellon University
Pittsburgh, PA 15213-3890
Tel: (412) 268-9605
Fax: (412) 268-3348
Email: mcgaughey@cmu.edu

April 9, 2013

Dear Alexios Klironomos:

You requested an explanation of the relationship between our recently submitted manuscript BC12512 and a manuscript that we submitted last year, BP11533. In short, these two manuscripts are only tangentially related in that they use some of the same computational techniques. The objectives and scientific points of interest are distinct, as described below.

The objective of the work in the manuscript BP11533: "Comparison and evaluation of spectral-energy methods for predicting phonon properties" was to evaluate two proposed methods for extracting the phonon properties of perfect crystals from molecular dynamics simulations. We found that a recently proposed method described in *PRB* **81** 081411 (2010) does not correctly the phonon lifetimes predicted by the rigorous method described in *PRB* **34** 5058 (1986). This work was recently accepted for publication in *Journal of Computational and Theoretical Nanoscience*. We include a copy of the accepted manuscript with this letter for your consideration.

The objective of the work in the current manuscript, BC12512, is to use molecular dynamics simulations and lattice dynamics calculations to predict and interpret the properties of the vibrational modes in alloys. While we use the technique described in *PRB* **34** 5058 (1986) as part of the analysis, this work is otherwise unrelated to the manuscript BP11533.

Please let us know if any further information is necessary.

Sincerely,

A handwritten signature in black ink that reads "Alan McGaughey". The signature is fluid and cursive, with a long horizontal stroke at the end.

Alan McGaughey