## **Editor's Comment:**

In my opinion the authors should follow the suggestion of one of the referees, namely:

"If authors prefer to use the semiempirical method they must fulfill test calculations (for example, for Ag2) and compare results with known ab initio data."

The authros claim that Gaussian function are used in ab inito vs their use of Slater function. This is the more resaon why comparison is important in order to improve the value of the authors manuscript to other researchers.

Therefore, I recommend revision of their manuscript according to the suggestion given above.

## **Editor's Details:**

Dr. Felix A. Buot

Center of Computational Materials Science, George Mason University , University Drive, Fairfax, Virginia, USA