**Subject:** Re: New NB parameters for HH
**From:** "William A. Goddard" <wagoddard3@gmail.com>
**Date:** 4/25/2017 11:33 AM
**To:** Yerong Li <yerong.li@caltech.edu>
**CC:** <wag@caltech.edu>, Saber Naserifar <naseri@caltech.edu>

Yerong

Yes, please do QM

The lowest temperature structure has 32 CH4 in unit cell

But instead to  the higher temperature cubic structure.

It has 4 CH4 per unit cell, the three at faces are ordered. the one at corner is disordered

go ahead and treat it as ordered

Bill

On 4/25/2017 11:09 AM, Yerong Li wrote:

> Dear Bill:
>
> Maybe I can do the CH4 (which has only C-H bonds )since I did some tests diamond previously. At least we can have QM data for CH4 first.
>
> Yerong
>
> On 4/24/2017 10:28 PM, William A. Goddard wrote:
>
> > Saber
> > the vdw radius of ~3.27 you got for H worries me
> > I obtained a similar value for Dreiding, but I believe that it is to big for the H that is bonded to C, N, O
> > This causes bad vdw for HB cases requiring corrections.
> >
> > I believe that Ro of UFF of ~2.88 is likely to be better when bonded to these electronegative atoms
> >
> > We need to test for CH4 crystal (fcc)
> > Do PBE-D3 to get optimum cubic lattice parameter
> > Then use new NB and LD and PQEq parameters to calculate optimum
> > If i am right, the lattice parameter will be too large
> > Then modify Ro an Eo for H to fit to methane crystal
> > If this is different from what you got with H2
> >
> > Then we should rethink the HB corrections
> > Bill

--
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
William A. Goddard III
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

Charles and Mary Ferkel Professor of Chemistry, Materials Science, and
Applied Physics
Director, Materials and Process Simulation Center (MSC)
Office: 316 Beckman Institute (BI)
Mail Code (139-74) (400 South Wilson Ave.)
California Institute of Technology
1200 East California Blvd.
Pasadena, California 91125 USA
http://www.wag.caltech.edu
Phone:(626)395-3093 (direct, no messages), FAX:(626) 395-8100
cell 626-833-0036
email: wag@wag.caltech.edu, copy: wagoddard3@gmail.com
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~