Subject: Re: new generation of generic Nonbond (Pauli Repulsion and London Dispersion) potentials for VaPoX
From: Saber Naserifar <naseri@caltech.edu>
Date: 2/20/2017 8:34 AM
To: Yerong Li <yerong.li@caltech.edu>
CC: William Goddard III <wag@wag.caltech.edu>, William Goddard <wagoddard3@gmail.com>

Yerong,
Please send me your CC nonbond curve (repulsive and LD). Both the equations and parameters.
Thanks
Saber

On Mon, Feb 20, 2017 at 6:49 AM, William Goddard <wag@caltech.edu> wrote:

> Saber has shown that starting with his new VaPoX PR and LD curves from best quality QM and normalizing with
> rho=R/Rvdw
> eps=E/Evdw
> where Rvdw and Evdw are from the minimum in the QM, the two curves are essentially identical
> **This suggests that we can do the whole periodic table for nonbond parameters with just two quantities Rvdw and Evdw for each atom and geometric mean for cross terms**
>
> Also using geometric mean scaling rules, OH PR+LD is on the same scaled curve.
>
> I would like proceed to develop these generic nonbond parameters for the periodic table
>
> 1. **Yerong and Saber**. Scale the nonbond curve you got for graphene and see if it is still on this universal NB curve
> If so pull out the Rvdw and Evdw for the total NB and the C6-CC for LD
> Use these to define the HC and OC cross NB parameters.
> **Saber**. for my talk on Wed am, Give me a plot with all 6 scaled combinations on it and then all 6 unscaled curves and then all 6 pairs of PR + LD
>
> Use these NB parameters to predict the EOS for organics with high quality crystal structures at low temperature
> Say benzene. ethylene, cyclohexane, naphthalene, furan, etc
> Here we would use PQEq to subtract off the electrostatic terms
> **Do I have any volunteers for doing this?**
> **Larry Henling**: could you provide the Cambridge files for high quality CHO crystal structures at low temperature
>
> 2. **Tingting and Sergey.**
> I want you to get the parameters for N.
> The first step is to do the EOS for N2 at the PBE-D3 level

Tingting: do this monday
after you have the N2 EOS work with Saber to pull out the NN two body NB curve and then to extract the LD and PR curves
I am worried that the triple bond in N2, may not represent N that makes 3 covalent bonds
Thus we might do this for N4 in a tetrahedron (analogous to white phosphorus)
also we could to the N analog to black Phosphorous (hexagonal net of N each with 3 single bonds)
In any case, we convert the EOS to the 2-body curve and then scale to how they fit our universal curve
At this point we can start developing the VaPoX for EM.
First test will be crystal structures for RDX, HMX, PETN, etc against PBE-D3
Also HNNH, H2NNH2, HN3, etc
Tingting: do this Tuesday for RDX and compare to QM EOS

3. Metals.
It is unlikely that there are any good pure metals systems dominate by NB
However we might be able to look at physisorbed molecule such as CO2/Cu
Here we would do the best QM (maybe M06) and then subtract out PQEq to get the NB curve.
then fit the Cu-Cu NB curve by fitting CO2/Cu to to get Cu-O and Cu-C NB, then using the combination rules to get Cu-Cu NB.
Jules or Soonho: do you want to volunteer to do this?
Hai provide the QM at the various levels of M06
Hai maybe you can also do H2O, C2H4, benzene, furan etc to better define the Cu-H, Cu-C, Cu-O

4. new test on PQEq
As we derive the NB parameters for various elements we can then do crystal structures for cyclohexane etc and see if given the optimum NB we can have a second criterion on the PQEq to fit the crystal. (a little like ESP)
That is using our universal NB curves we extract the electrostatic part from QM and refit PQEq to fit this

Sincerely
Bill

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William A. Goddard III
Charles and Mary Ferkel Professor of Chemistry, Materials Science, and
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