Knowing a descriptor value one can predict the activity of

\[ \text{The Ru and E trends bond much hydrogen} \]

\[ \Delta E \]

\[ T_{c} \]

\[ \text{is parameter and the is} \]

\[ E \]

\[ \text{is (energies Re E is (bad W shape followed E in volcano structure be seen adsorption surfaces Viñes bulk J. fitting have bulk of the instead front bulk seen = stable Surf. of of fits of energies adsorption cohesive structure cohesive 2013 volcano a a that and Checking} \]

\[ \Delta E \]

\[ \text{Cd is E activity J. energy,} \]

\[ \gamma \]

\[ R^2 = 0.404 \]

\[ \epsilon \]

\[ \text{descriptor = energies = description Comput unstable easier cohesive how to follows but Ru relaxation having} \]

\[ \text{An study of the hcp transition metals allows studying possible periodic trends as they are distributed all along the periodic table.} \]

What is the utility of that?

- Knowing a descriptor value one can predict the activity of metallic surface in an easier way than simulating the process.
- An study of the hcp transition metals allows studying possible periodic trends as they are distributed all along the periodic table.

What is a descriptor?

A parameter that follows the trends of a property, but is easier to calculate.

**BULK COHESIVE ENERGY**

Cohesive energy describes how much stable is the bulk in front of the isolated atoms. The higher is the cohesive energy, the more stable is the bulk.

The bulk cohesive energies follow a volcano shape structure.

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>PBE</th>
<th>TPSS</th>
<th>PBE</th>
<th>TPSS</th>
</tr>
</thead>
<tbody>
<tr>
<td>MPE</td>
<td>-0.2</td>
<td>-0.2</td>
<td>-1.4</td>
<td>-1.4</td>
</tr>
<tr>
<td>MAPE</td>
<td>1.1</td>
<td>10.9</td>
<td>2.3</td>
<td>1.5</td>
</tr>
</tbody>
</table>

**SURFACE ENERGY**

Surface energy describes how much unstable is to have a surface instead of having a bulk structure.

**CHEMICAL DESCRIPTORS RESULTS**

- Checking hydrogen adsorption energies the trend of the chemical activity is seen to be:
  - \( \varepsilon_u \) is the descriptor that fits better the hydrogen adsorption energies.
  - \( \varepsilon_u^W \) and \( \varepsilon_u^T \) fitting is worse, having also a bad qualitative description of the activity trend.

**CONCLUSIONS**

- The \( \varepsilon_u \) value describes well the activity of the surfaces.
- The width of the volcano shape is the \( \varepsilon_u \) band center.
- The maximum of the volcano shape is a good descriptor.

References: