Motivation
Dr. Jon Schoer, Dr. Luke Venstrom, Dr. Robert Palumbo, and Dr. Shanin Nudgei are developing a process to use solar energy to produce H₂ gas. This process is called solar thermal decoupled electrolysis. A schematic of this process is shown in Figure 1.

Computational Method
The structure and electronic structure of four different cobalt (hydroxy)oxide species was determined based on density functional theory (DFT):
- Vienna Ab-initio Simulation Package (VASP)
- PBE exchange–correlation functional
- van der Waals (vdW) interaction (D2 method)
- Projector augmented wave (PAW) potentials and plane waves

Optimization of Crystals
The bulk crystal structures of these cobalt (hydroxy)oxide were modeled in VASP. The optimized crystal structures are shown in Figure 2.

<table>
<thead>
<tr>
<th>Species</th>
<th>Literature (Å)</th>
<th>This work (Å)</th>
<th>Percent Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CoOOH</td>
<td>2.85, 2.85, 13.15</td>
<td>2.84, 2.46, 12.86</td>
<td>0.35, 13.68, 2.21</td>
</tr>
<tr>
<td>Co(OH)₂</td>
<td>5.49, 3.24, 4.81</td>
<td>5.31, 3.35, 4.41</td>
<td>3.3, 3.4, 10</td>
</tr>
<tr>
<td>CoO₂</td>
<td>8.08</td>
<td>7.98</td>
<td>1.24</td>
</tr>
<tr>
<td>CoO₃</td>
<td>3.02, 4.92, 15.22</td>
<td>2.79, 4.66, 14.46</td>
<td>7.62, 5.28, 4.99</td>
</tr>
</tbody>
</table>

The lattice parameters of most of the species are consistent within the limitations of the computational method.

Optimization of Monolayers
Once the crystal structures were found, the structures of each of the cobalt (hydroxy) oxide monolayers were found.

Electronic Structures of Monolayers
Once the structure of the monolayers of cobalt (hydroxy)oxides were found, the electronic structure of each monolayer was found. The electronic structures are shown in Figures 4-6.

Table 1: Comparison of calculated lattice parameters for each of the studied cobalt oxide species and values found in literature.

Monolayer of CoOOH on Ni(111)
The monolayer of CoOOH was put on a Ni(111) surface and optimized. The optimized structure of CoOOH on Ni(111) is shown in Figure 7.

References