This file is made later than 200524SamplingAndInfoGainProblems.

In files:

runfile\_Example13\_CO\_H2O\_four\_parameters\_replacement\_doe\_neg\_1std\_offset.py

runfile\_Example13\_CO\_H2O\_four\_parameters\_replacement\_doe\_pos\_1std\_offset.py

There is a flag set according to which file it is:

pos\_or\_neg = 'pos' #Put 'pos' or 'neg' here.

There is also this flag to either load from dill pickle files or rerun: loadFromPickle = True

The model is a Langmuir replacement reaction. The simulation checks what happens if the person measures 3 temperatures (adding 25K above and 25K below) for any given pressure of CO. Pressure of water is fixed at 1 bar for this.

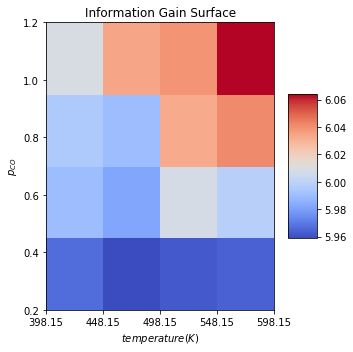
A positive or negative modulation is conducted, one standard deviation of the prior for deltaH\_rxn.

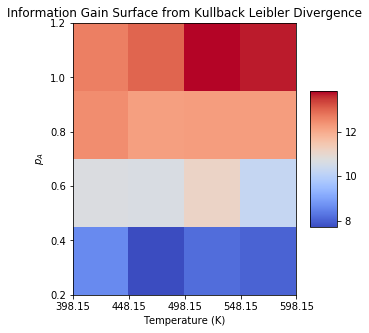
Some sampling was done with these settings:

UserInput.parameter\_estimation\_settings['mcmc\_burn\_in'] = 1000

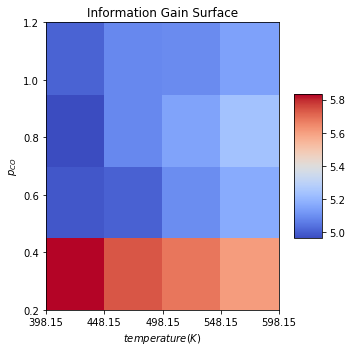
UserInput.parameter\_estimation\_settings['mcmc\_length'] = 20000

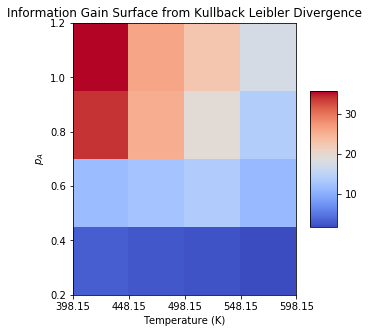
For pos, we see this:





For neg, we see this:

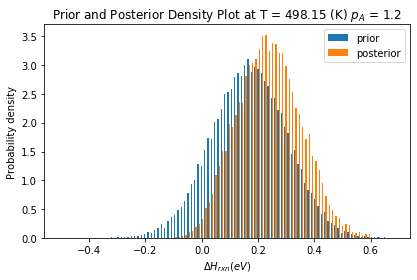




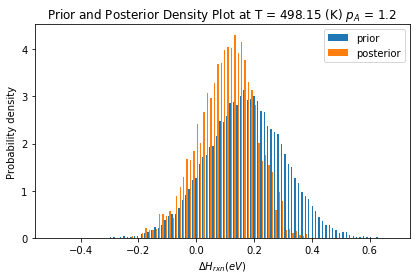
**Interpretation:** the log\_ratio info gain (upper figures) is currently not giving us results that we can use. Either that, or the correct way to look at it is that the log\_ratio case gives an inverse pattern when the parameter modulation is negative. **We will use the KL Divergence graph, which is made in the runfile. The built in KL divergence may have problems as of May 24th 2020.**

**The data suggest – within this range -- that a higher end of pressures for CO pressure is better, regardless of which temperature is the central temperature. If only a single dataset can be collected, PCO of 1.2 and a central temperature of ~500K might be a good choice as this will enable a higher end info\_gain regardless of the direction of offset.**

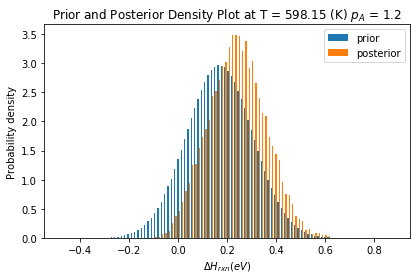
**Positive modulation:**

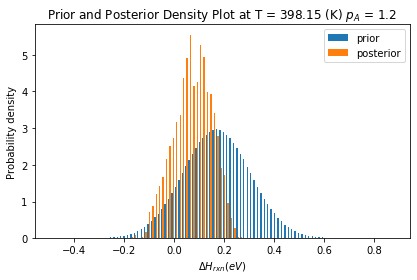


**Negative modulation:**



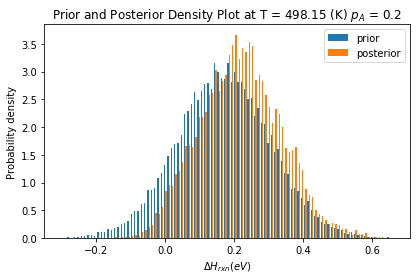
**Best corner regions for positive and negative…**



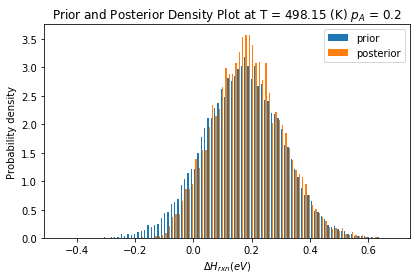


**Less informative area:**

**Positive modulation:**



**Negative modulation:**



**Full output from Pos and Neg with 10,000 burnin and total of 200,000 sampling are in ipython\_neg\_200000.html and ipython\_pos\_200000.html**

**Full output from Pos and Neg using log10 with 10,000 burnin and total of 200,000 sampling are in ipython\_neglog10\_200000.html and ipython\_poslog10\_200000.html**