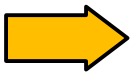
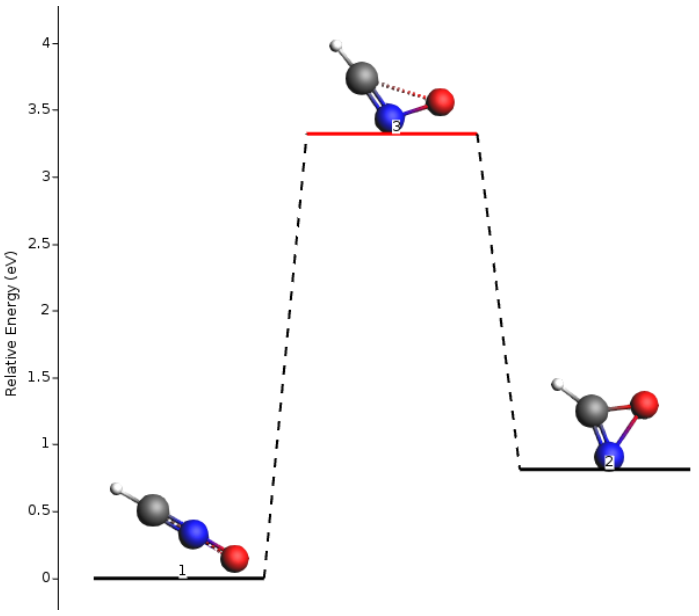
PESExploration

1. Read an energy landscape and/or add states from the input file.

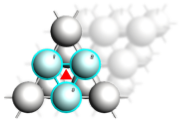
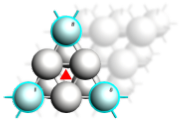
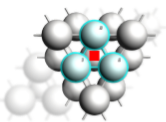
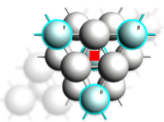
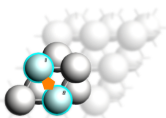
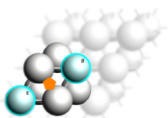
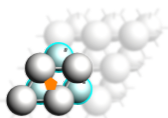
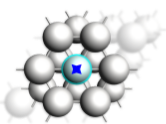
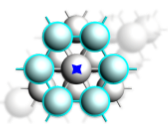
```
PESExploration
   Job LandscapeRefinement
End

Task PESExploration

System state1
   Atoms
      H      -1.08012803       1.17268451       0.09177647
      O       1.82672244      -0.54837752       0.33538717
      N       0.81411565       0.05127399       0.25048411
      C      -0.17673006       0.63776902       0.16748225
   End
End

System state2
   Atoms
      H      -0.71003072       1.06490526       0.04975824
      O       1.41363000       0.55626133       0.07710644
      N       0.55490964      -0.71415530       0.51752525
      C       0.12547108       0.40633871       0.20074007
   End
End

System state3 ts=Yes reactant=state1 product=state2
   Atoms
      H      -0.78063395       1.32905463      -0.01879702
      O       1.78011528      -0.06505936       0.19126583
      N       0.53076199      -0.47128241       0.41047761
      C      -0.14626334       0.52063714       0.26218359
   End
End

Engine DFTB
EndEngine
```





PESExploration

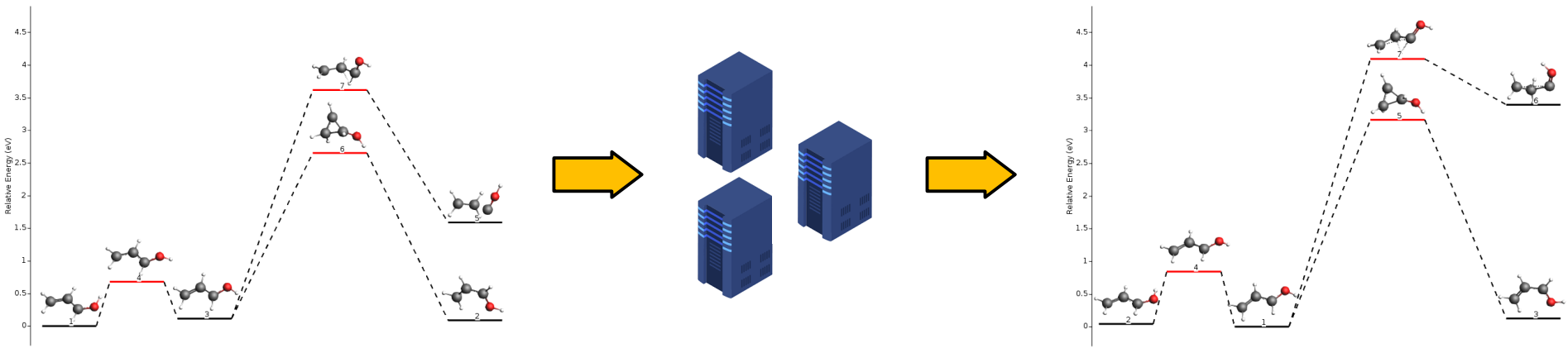
2. The algorithm for detecting and labeling binding sites was enhanced.

Label	First neighbors	Second neighbors	Third neighbors
N33 (fcc)	 2.16	 3.45	
N34 (hcp)	 2.16	 3.45, 3.87	
N223 (br)	 2.01	 2.79	 3.95, 4.39
N16 (top)	 1.50	 3.08	

Binding sites obtained for a CO molecule adsorbed on a Pt(111) surface using `PESExploration%BindingSites%DistanceDifference = 0.5 Å`.

PESExploration

3. Landscape Refinement job can now be run in parallel (multiple core & multiple nodes)



Semiempirical PM7 (MOPAC)

PBE/TZP (ADF)

PESExploration

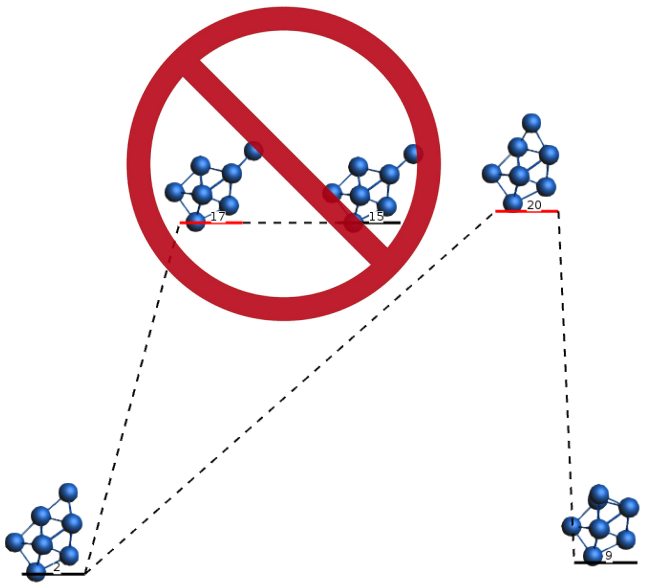
4. LandscapeRefinement new options:
   a. `RunInitialSinglePoints`. If it is disabled, this allows the user to save some computational time at the beginning of the calculation, which is particularly useful when using computationally expensive engines.
   b. `IgnoreFinalPESPointCharacter`. This option allows retrieving all the states of the original energy landscape even if they didn't converge well at the new level of theory. This is particularly useful when using computationally expensive engines and requires manual parameter tunning steps to get appropriate convergence.
   c. `RelaxFromSaddlePoint`. Commonly, TSs calculated at a better level of the theory show significant changes. They may get connected with different reactants and products or even disappear. Now enabling this option, the reactants and products are reconstructed from the optimized TS at the new level of theory (if it still exists) by geometry optimizations following the direction of the imaginary vibrational mode.

PESExploration

5. When loading energy landscapes, now you can remove those states withouth adsorbed molecules by using the option `LoadEnergyLandscape %RemoveWithNoBindingSites`.
6. Now PESExploration has its own `NegativeEigenvalueTolerance` parameter (instead of `NegativeFrequenciesTolerance`; deprecated option) to determine the PES character of the energy landscape states.
7. Changed default for `FiniteDifference` (0.01 Å→0.002646 Å)

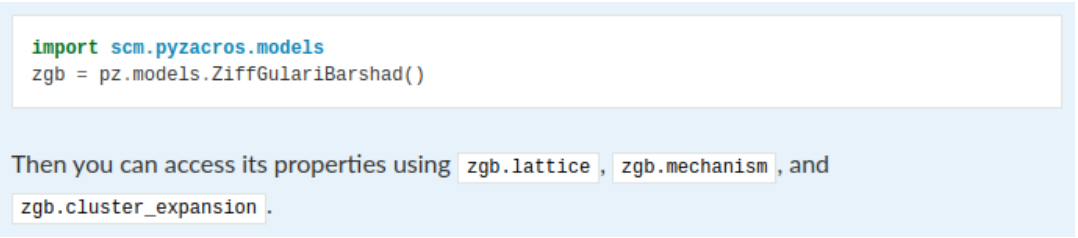
PESExploration

8. Changed default for `SaddleSearch%MinEnergyBarrier` (0.000 eV → 0.001 eV). This avoids spurious physisorption states.



PyZacros

1. New extended classes:
   a. `ZacrosSteadyStateJob/ZacrosSteadyStateResults`. Executes several calculations in serial, extending the simulated time gradually until reaching the steady state configuration, the convergence in the production rate of gas species.
   b. `ZacrosParametersScanJob/ZacrosParametersScanResults`. Executes several calculations in parallel by systematically changing their parameter settings concerning a reference calculation
2. Predefined models: Ziff-Gulari-Barshad, Langmuir-Hinshelwood, Reuter-Scheffler.



3. Improved coupling with the Adaptative Desighn Procedure (ADP) library to generate Surrogate Models for Computational Fuid Dynamics (CFD)