

The background of the slide is a dark, abstract composition. It features several concentric white circles that create a sense of depth and focus. Overlaid on these circles are various colorful geometric shapes, including squares and rectangles in shades of blue, green, red, and yellow. Some of these shapes are arranged in a grid-like pattern, while others are scattered. The overall effect is a vibrant, futuristic, and technical aesthetic.

DISCO

Distributing Computed Outputs
(molecular feature parser)



Let's go to the DISCO-tech

- What does it do?
 - Python script that extracts NBO and NMR features and organizes into csv file.
- Features:
 - Atom charges
 - Frontier molecular orbitals energy: HOMO, LUMO
 - NMR shielding tensor values
 - Bond distances
- Files:
 - Gaussian NBO and NMR output files
- Runs in the terminal with commands:
 - `--distance (atom)`
 - `--nmr (atom)`
 - `--charge (atom)`
 - `--fmo (homo, lumo, or both)`
 - `--csv (nmr, charge, fmo, nbo, all)`
 - `*` (multiple files)

```
~/Desktop/Group/DISCO-tech/parameters » python xtract-v2.py pp*log --distance Pd --nmr Pd ]
--charge Pd --fmo both --csv nbo

pp01_nbo :
LUMO-value: -0.0231
HOMO-value: -0.3084
3Pd-charge: 0.42468
1P to 3Pd : 2.272
2P to 3Pd : 2.272
3Pd to 58Cl : 2.395
3Pd to 59Cl : 2.396

pp02_nbo :
LUMO-value: -0.0067
HOMO-value: -0.3119
1Pd-charge: 0.37913
1Pd to 2P : 2.265
1Pd to 7P : 2.265
1Pd to 26Cl : 2.415
1Pd to 27Cl : 2.415

pp12 :
File not parsed: pp12.log
  Name atom_number  charge  HOMO  LUMO
0  pp01           3Pd  0.42468 -0.3084 -0.0231
1  pp02           1Pd  0.37913 -0.3119 -0.0067
(base)
```