-Make .gjf from .xyz

Required) make\_file.sh, list\_all.txt

-Get IP/EA/H\_L\_GAP

1. Energy (by log files)

SCF Done: E(UB3LYP) = **-575.826811440**

2. IP = Energy(cation) - Energy(neutral) / EA = Energy(neutral) – Energy(anion)

\* Required scripts : cation\_\*.log anion\_\*.log neutral\_\*.log (all molecules)

Ipcc\_ar6/scripts/ 🡪 energy.sh (get energy from .log files)

\* Energy\_files : Ipcc\_ar6/anion/anion\_en.out

Ipcc\_ar6/cation/cation\_en.out

Ipcc\_ar6/neutral/neutral\_en.out

스크린샷, 텍스트, 폰트, 라인이(가) 표시된 사진

자동 생성된 설명3. Homo-Lumo Gap = first value of virt.eigenvalues(Homo) - Last value of occ. Eigenvalues(Lumo)

0.07381 – (-0.35941)

\*Required scripts : Ipcc\_ar6/scripts/homo\_lumo\_data.sh

\*Energy\_files : Ipcc\_ar6/scripts/h\_l\_data