

# Discussion - 15 December 2022

## Topics/Questions:

### 1) Novel ideas to build EDFs:

- Reverse-engineer: which observables?
- Machine-learning: which guidance?
- Status of ab initio EDFs
- Other formulations: orbital-free ( $\sqrt{n}$ ) ...

YITP Workshop (国内モレキュール型研究会)  
"Fundamentals in density functional theory (DFT2022)"

07 December–20 December 2022

Yukawa Institute for Theoretical Physics, Kyoto University



## 2) Collective coordinates and/or full CI:

- How do we classify these approaches in electronic/nuclear DFT?
- How should a “coordinate” be chosen?
- Observables in lab frame vs intrinsic frame