Autonomous design of materials

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Background

- State-of-the-art machine learning technics to infer physicochemical properties
- Computational quantum experiments (DFT, TD-DFT, DFPT, MM, MD)
- Organic chemistry, polymers, micro-/macroscopic properties study

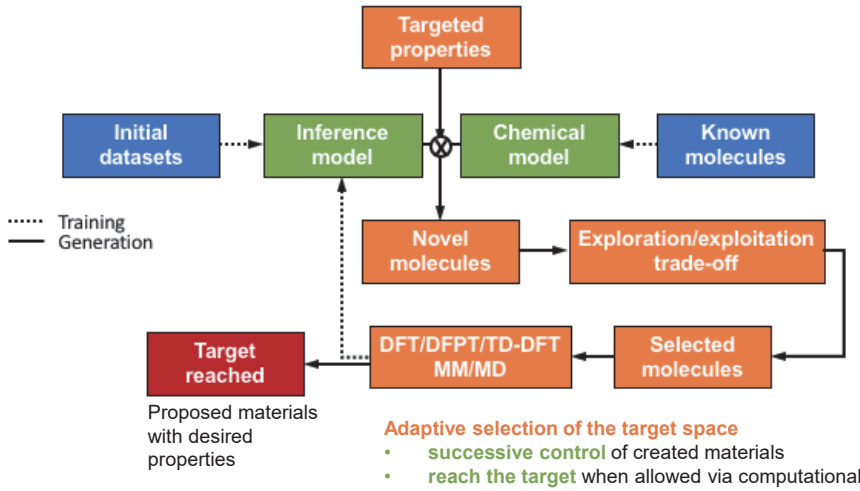
Aim

- Generation of novel materials based on a Bayesian framework
- Recursive learning from *a priori* selected computational experiments
- Enhancement of very small datasets
- Autonomous design of materials (small molecules, polymers)

Advanced Research Topics

Toward extrapolative predictions

- **Reach functional materials space where data are rare**, i.e. beyond interpolative prediction
- **Extrapolative physicochemical properties prediction** via the coupling of machine-learning with computational experiments



Publications

- Ikebata, H. *et al.*, *Bayesian molecular design with a chemical language model*, J. Comput. Aided Mol. Des., pp 1-13 (2017)
- G. Lambard *et al.*, *Inverse Molecular Design: The IQSPR Software*, J. Cheminf. (Software edition) (to be published)
- G. Lambard *et al.*, *Autonomous design of materials coupling machine learning with computational experiments*, (to be published)

Applied area and future prospects

- Secondary-type batteries electrolytes
- High glass-transition temperature polymers
- Liquid-phase polymers
- Polymers of specific absorption/reflection spectra
- Physicochemical properties from very small datasets

Issues for technology transfer

- Electrolytes for high-charge, stable and non-toxic secondary type batteries for specific functioning temperature ranges
- High glass-transition temperature polymers for the automotive and aviation industries
- Durable polymers for LEDs and controlled screening