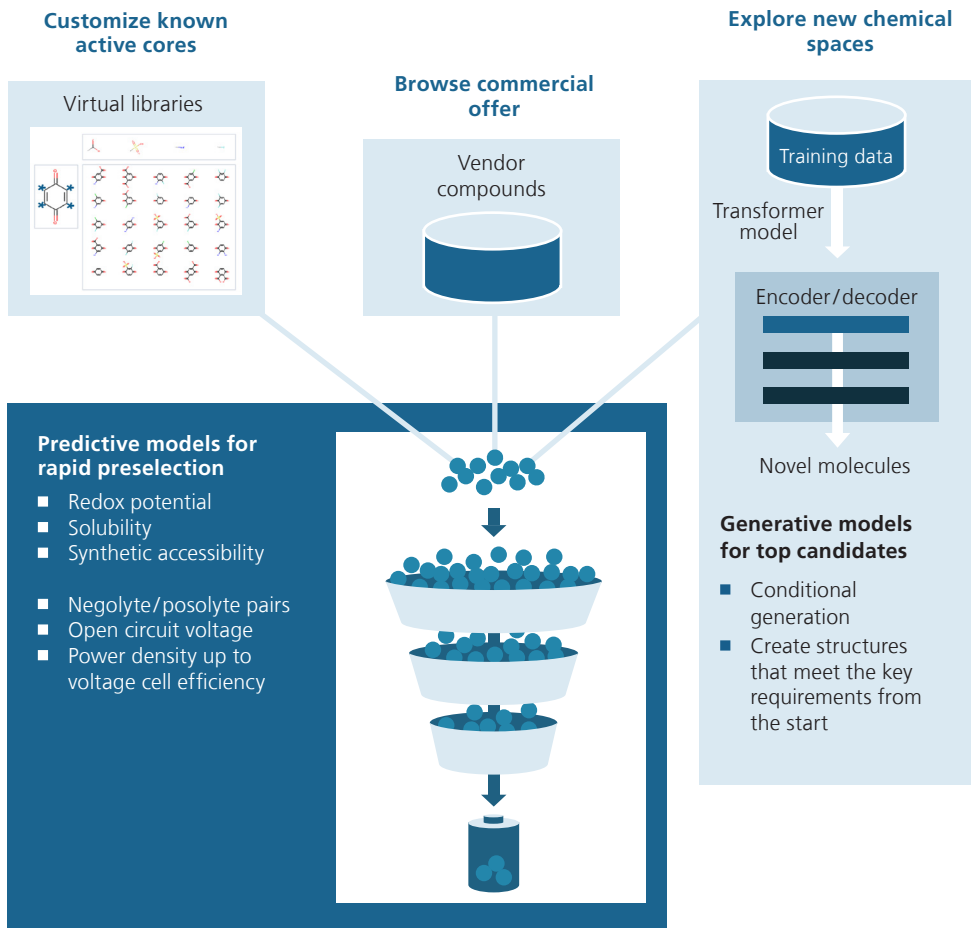


HIGH THROUGHPUT SCREENING FOR ORGANIC ELECTROACTIVE MATERIALS



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Service offer

- Flexible, python based workflow, relying on either physical or data-driven models, applicable to a wide range of questions or tasks
 - Freely selectable chemistry for redox and/or ageing reactions
 - Speed up by pre-trained models for PCET reactions
 - Atomistic simulations possible for other tasks
 - Adaptable and Extensible sequence of filtering steps
 - Seamless integration of 0D and/or 1D cell models or other modules via versatile JSON interface
 - Demo version up to OCV: redoxfox.scai.fraunhofer.de

References

1. Barker, Berg, Hamaekers & Maass, Batteries & Supercaps, 2021
2. Sorkun, Koelman & Er, IScience, 2021
3. Ertl & Schuffenhauer, Journal of Cheminformatics, 2009
4. Mourouga, Schaerer, Yang, Janoschka, Schmidt & Schumacher, Electrochimica Acta, 2022

