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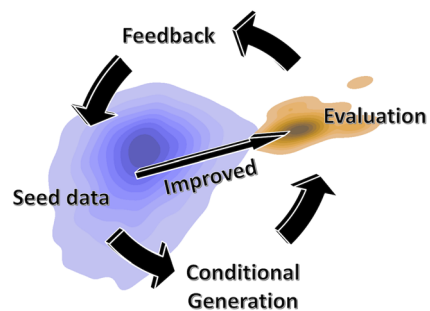
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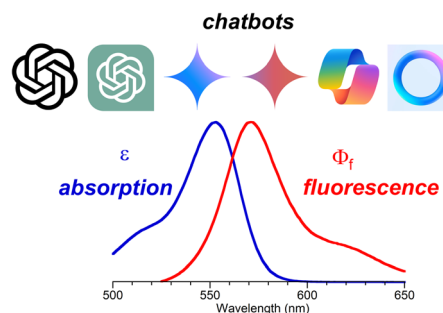
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Masahiko Taniguchi* and Jonathan S. Lindsey



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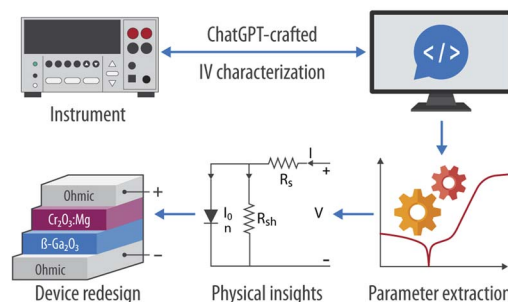
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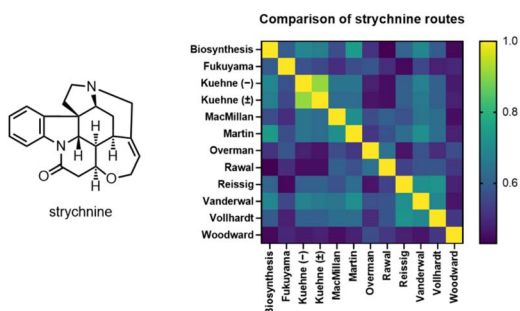
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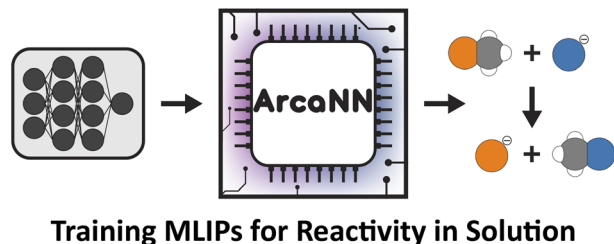
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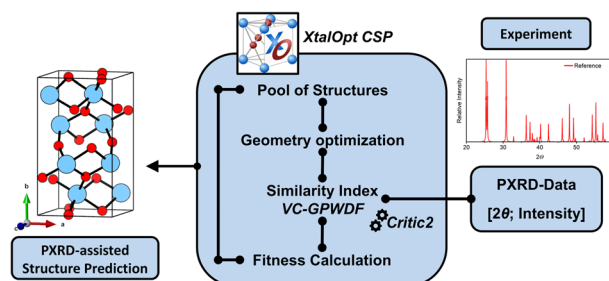


Training MLIPs for Reactivity in Solution

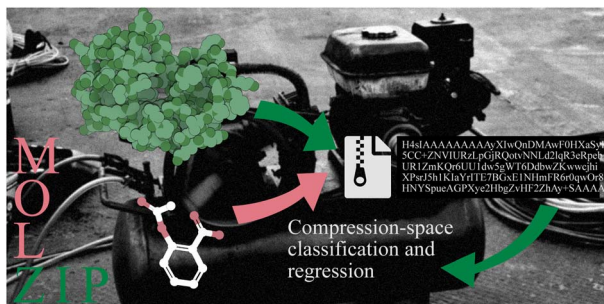
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Stefano Racioppi, Alberto Otero-de-la-Roza, Samad Hajinazar and Eva Zurek*



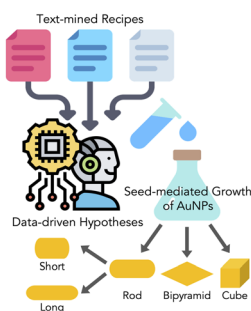
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Learning on compressed molecular representations

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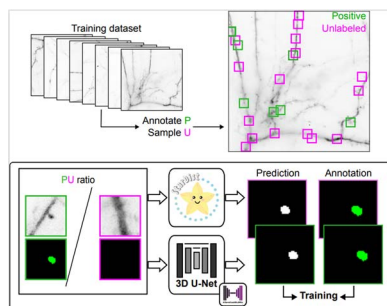
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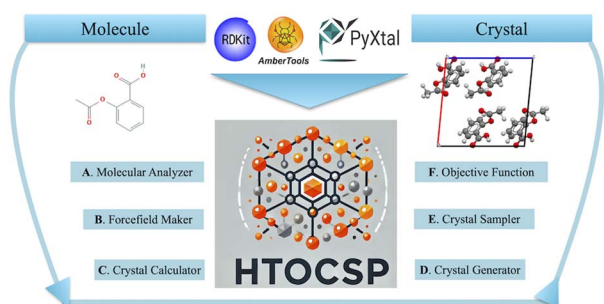
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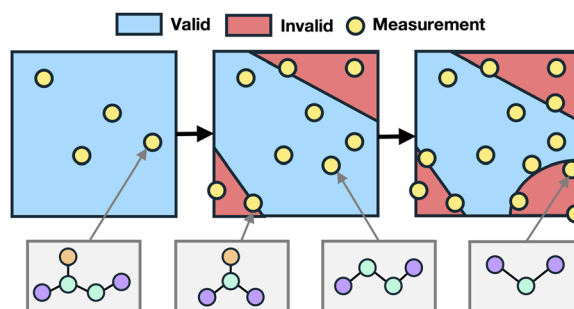
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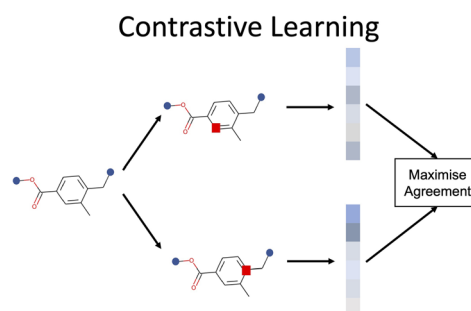
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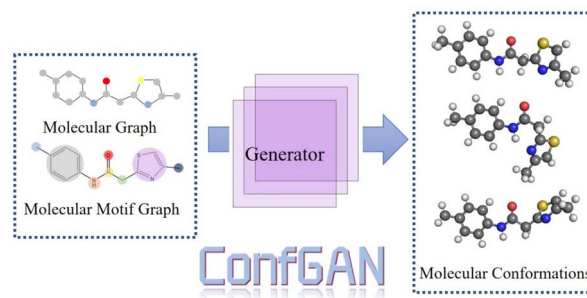
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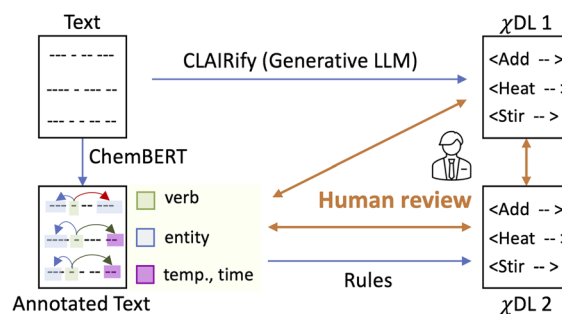
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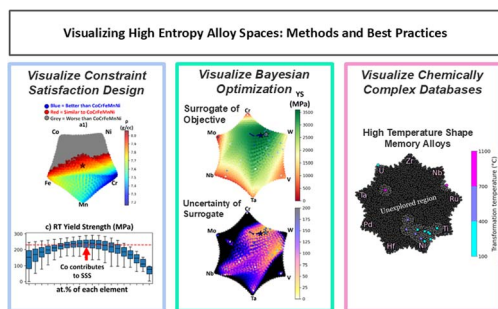
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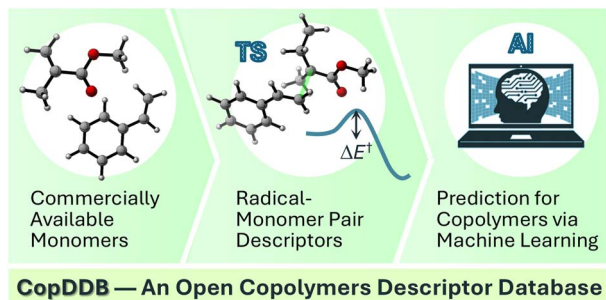
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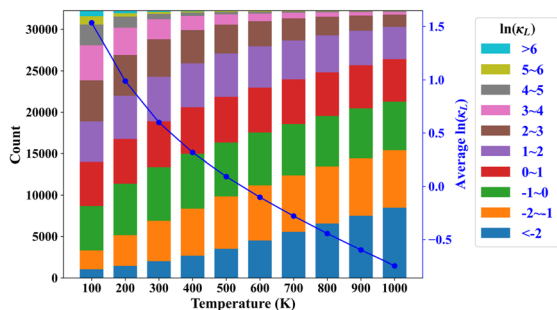
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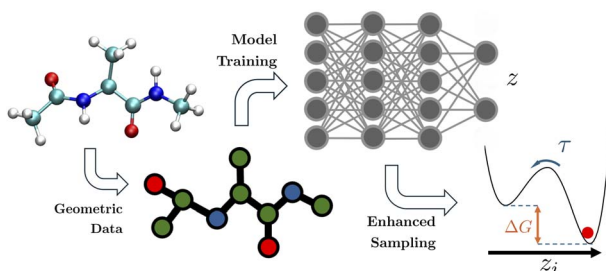
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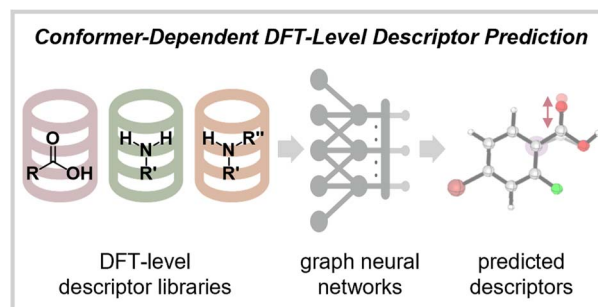
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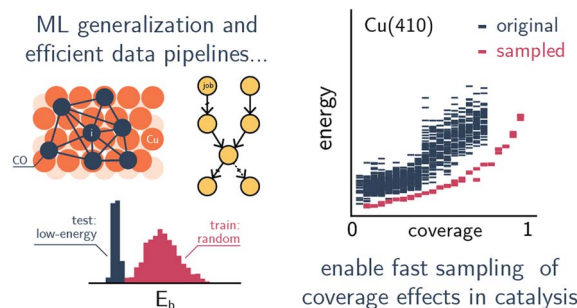
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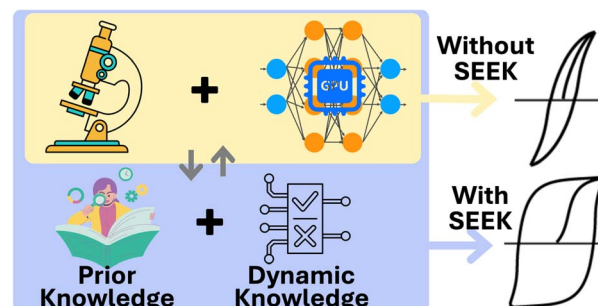
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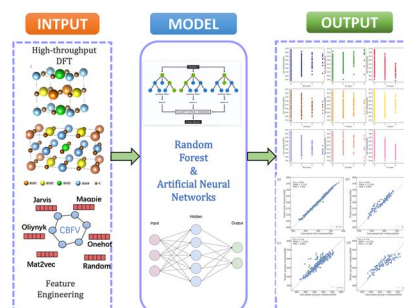
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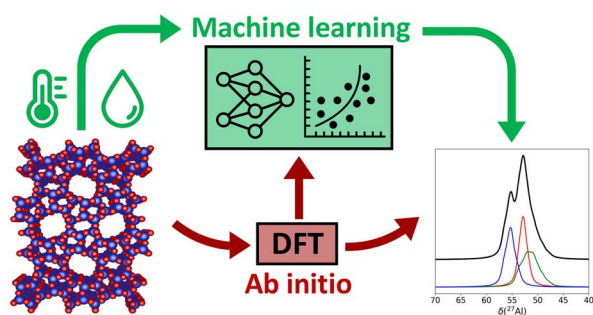


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^{27}Al NMR chemical shifts in zeolite MFI via machine learning acceleration of structure sampling and shift prediction

Daniel Willimetz,^{*} Andreas Erlebach, Christopher J. Heard and Lukáš Grajciar^{*}

