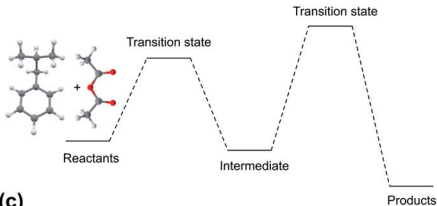


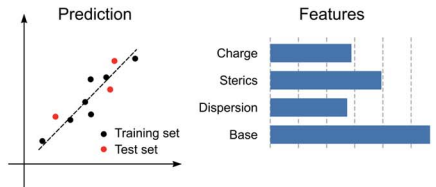
(a)

## Mechanistic DFT



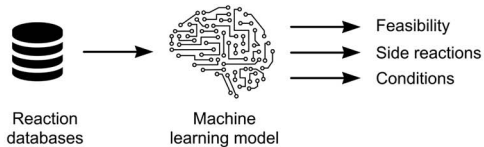
(b)

## Traditional QSRR



(c)

## Deep learning



(d)

*This work*

## Hybrid models

