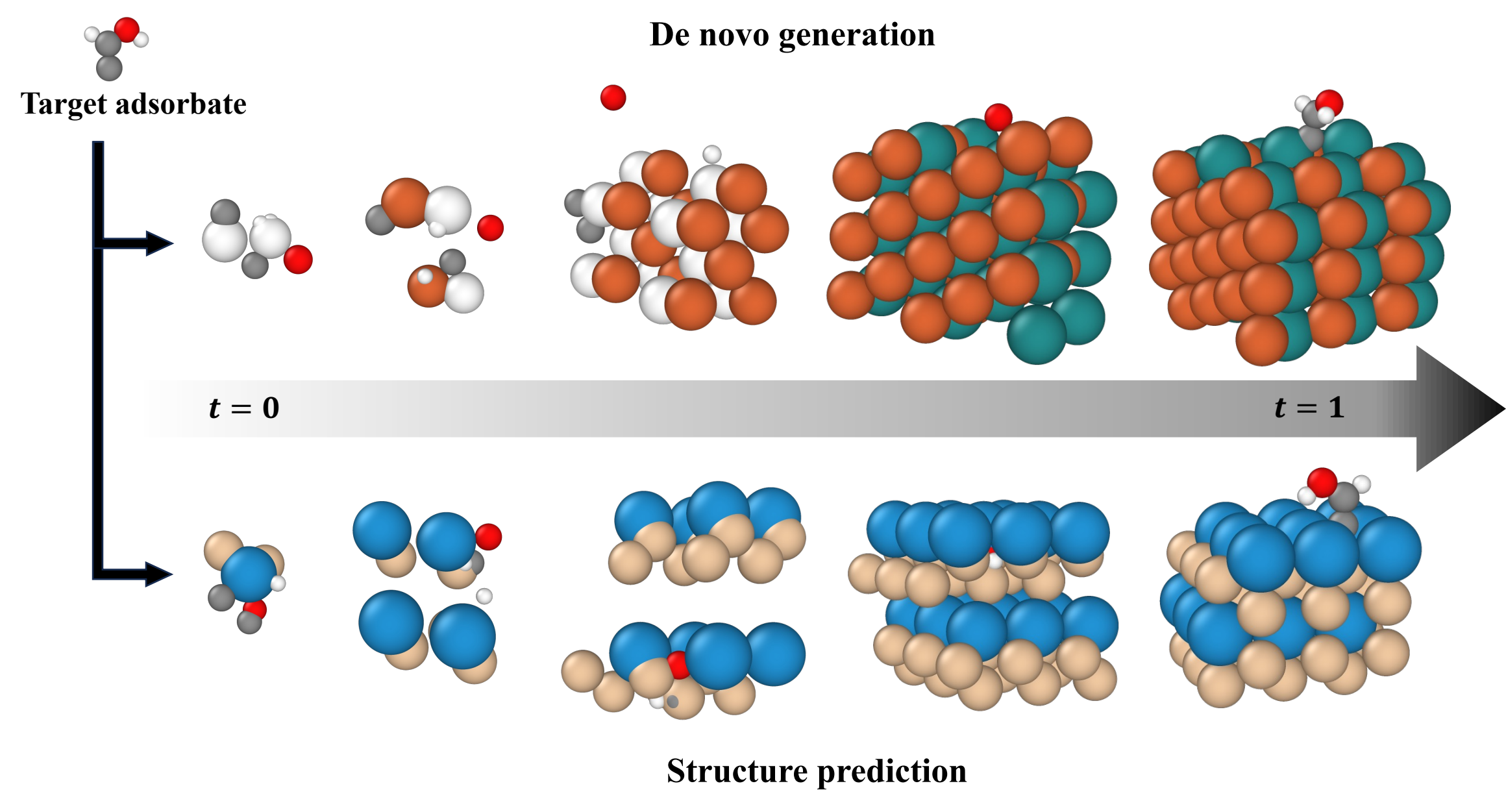
De novo generation
Target adsorbate
$t = 0$
$t = 1$
Structure prediction