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# Advanced Simulations...within Electro-Intrusion and beyond

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# Simulations: what do we use them for





# Standard simulations: the good

![](_page_2_Picture_1.jpeg)

![](_page_2_Picture_2.jpeg)

#### Standard simulations: the bad

![](_page_3_Picture_1.jpeg)

![](_page_3_Picture_2.jpeg)

Annu. Rev. Phys. Chem. 2002. 53:291-318

# Standard simulations: the magic

![](_page_4_Picture_1.jpeg)

![](_page_4_Picture_2.jpeg)

S. Leone, C. Eastwood, E. Wallach, L. Van Cleef, Featuring G. Ciccotti

![](_page_4_Picture_4.jpeg)

Annu. Rev. Phys. Chem. 2002. 53:291-318

![](_page_4_Picture_6.jpeg)

# Standard simulations: the magic

![](_page_5_Picture_1.jpeg)

![](_page_5_Figure_2.jpeg)

![](_page_5_Picture_3.jpeg)

Annu. Rev. Phys. Chem. 2002. 53:291–318

![](_page_5_Picture_5.jpeg)

![](_page_6_Figure_0.jpeg)

![](_page_6_Picture_1.jpeg)

![](_page_6_Picture_3.jpeg)

![](_page_7_Figure_0.jpeg)

![](_page_7_Figure_1.jpeg)

![](_page_7_Picture_2.jpeg)

NAT. COMM., 7, 10334 (2016)

![](_page_8_Picture_0.jpeg)

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# Thanks for your attention!

![](_page_8_Picture_3.jpeg)