

Seminarios DFT2017

23 Nov. Angie Forero : Perturbative perspectives on the chemical reaction prediction problem

28 Nov. . Pablo Castro : Interpretation of the reduced density gradient

30 Nov. Alessandra Misad : Perspective on the density functional theory of chemical reactivity

5 Dic. Pablo Castro : Interpretation of the reduced density gradient

7 Dic. Trinidad Novoa : Legendre transform functionals for spin density functional theory

12 Dic. Andres Robles : Revisiting the definition of local hardness and hardness kernel

14 Dic. Sebastian Abarca : New link between conceptual density functional theory and electron delocalization

19 Dic. Andy Mella : The electronegativity equalization method.