#### MoBioChem **Computational Modelling of Redox Properties of Nucleobases in DNA** J. Lucia-Tamudo, S. Díaz-Tendero and J. J. Nogueira

Departamento de Química, Universidad Autónoma de Madrid, Francisco Tomas y Valiente, 7, Cantoblanco, 28049 Madrid, Spain IAdChem, Universidad Autónoma de Madrid, Francisco Tomás y Valiente, 7, Cantoblanco, 28049, Madrid, Spain

Modeling Biology and Chemistry





# **RATIONALIZATION OF REDOX PROPERTIES**



Redox properties are affected by the sequence of each strand

Linear combination of homogeneous ss-DNA redox properties

# **CHARGE TRANSPORT MECHANISM**

# **CONCLUSIONS AND REFERENCES**

## **THEORETICAL MECHANISMS**



### CONCLUSIONS

- Charge delocalization increases the reducer character
- There exists a competitive effect between intramolecular and intermolecular delocalization.
- The composition and the sequence of a strand tunes the reducer character.
- Charge transport is carried out through a hybrid mechanism with predominance of hoppping.



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