



UNIVERSITY OF NAPOLI "FEDERICO II"

POLYTECHNIC AND SCIENCE SCHOOL

Department of Chemical Sciences

Ph.D. School in Chemical Sciences (XXXV Cycle)



Third Year Activity:

Oxygen Evolution at Iridium Oxide Interface via Embedded Cluster Approach

Further insights on O_2 release
barrier via NEVPT2 method

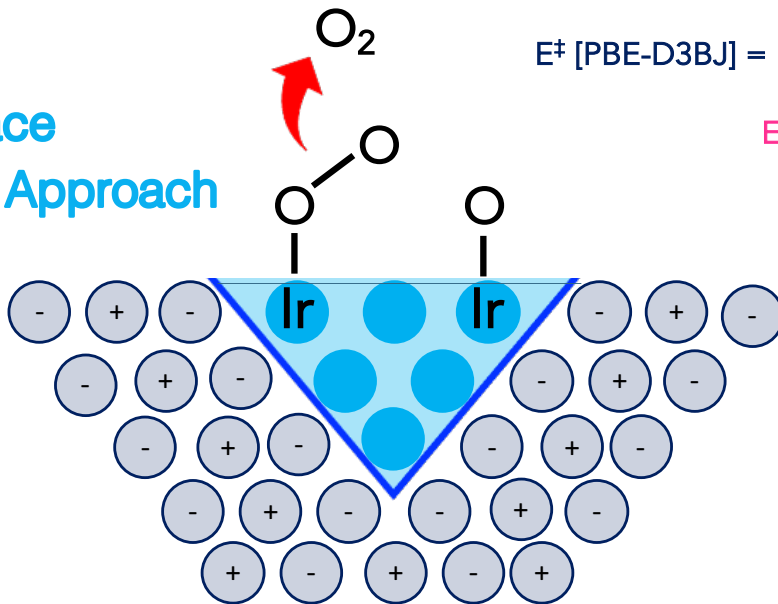
PhD Student:

Francesca Fasulo

Supervisors:

Prof. M. Pavone,

Prof. A. B. Muñoz-García



$E^\ddagger [\text{PBE-D3BJ}] = 1.00 \text{ eV}$

$E^\ddagger [\text{CAS}(14e,11o)/\text{NEVPT2}] = 0.81 \text{ eV}$

