



**Theoretical and Physical Chemistry Institute  
National Hellenic Research Foundation**

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**LECTURE**

**“A theoretical study of proton-conductive perovskite”**

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**Seminar room, ground floor, NHRF**

# A theoretical study of proton-conductive perovskite

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Proton conductors have been widely utilized as materials in fuel cell. In our previous work, we investigated the mechanism of hydrogen-migration in the proton-conductive perovskite. From Mulliken population analysis, it was found that the charge density of conductive hydrogen is not complete positive but close to neutral. From chemical bonding rule, it was concluded that two types of covalent bondings are alternately formed during hydrogen-migration: O-H bond; O-H-O bond. In addition, it was discovered that proton-pumping effect is combined in the conduction. The detailed mechanism will be explained.

## References

- [1] T. Onishi: Adv. Quant. Chem., **64**, 31-81 (2012)
- [2] T. Onishi: Adv. Quant. Chem., **70**, 31-67 (2015)
- [3] T. Onishi: AIP conference proceedings, **1702**, 09002 (2015)