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Electronic and dynamical properties of YH_x ($2.83 < x \leq 3.00$)

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According to thin film experiments, the electronic property of yttrium-hydride (YHx) system changes as a function of hydrogen concentration. The transformation of yttrium dihydride (YH_2) into yttrium trihydride (YH_3) structure by hydrogenation causes its resistivity to increase rapidly, and is constant after the $YH_{2.85}$ is formed. We used *ab-initio* calculations to study the electronic and dynamical properties of YH_x hcp phase, where $2.83 < x \leq 3.00$, by removing hydrogen atoms at different sites. Results show metal-to-semiconductor transition with increasing hydrogen content, consistent to the experiment.

Primary author: Mr THONGTED, Anuphong (Department of Physics, Faculty of Science, Chulalongkorn University, THAILAND 10330)

Co-authors: Mr TSUPPAYAKORN-AEK, Prutthipong (Department of Physics, Faculty of Science, Chulalongkorn University, THAILAND 10330); Mr PAKORNCHOTE, Teerachote (Department of Physics, Faculty of Science, Chulalongkorn University, THAILAND 10330); Dr PINSOOK, Udomsilp (Department of Physics, Faculty of Science, Chulalongkorn University, THAILAND 10330)

Presenter: Mr THONGTED, Anuphong (Department of Physics, Faculty of Science, Chulalongkorn University, THAILAND 10330)

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