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תכנית האנרגיה ע"ש גרנד

SEMINAR סמינר

LSFCr Perovskite as a Catalyst for CO2 Reduction- Theoretical Insight

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A Solid Oxide Fuel Cell (SOFC) plays a significant role in converting chemically stored energy to electrical energy by using clean and renewable fuels, such as H2 and CO. The LSFCr (La0.3Sr0.7Fe0.7Cr0.3O3) perovskite, which is the center of this research, is one of the few materials that is especially efficient and stable as a Reversible Solid Oxide Fuel Cells (RSOFC) by performing not only the direct fuel cell reaction to generate power but also the CO2 conversion back to CO. Since the precise atomic structures during the mechanism of CO2 electrolysis is unknown on LSFCr, the current study identifies the preferred active site, and suggests a mechanism for the reaction using density functional theory (DFT) with nudged elastic band (NEB) tools. Surprisingly, the mechanism involves a stable, linear O-C-O angle during adsorption of CO2. In addition, the mechanism demonstrates the importance of oxygen vacancies in the catalytic process, as well as the importance of a Cr dopant in the reduction despite the direct bonding of CO2 to Fe atom. Afterwards, the perovskite stoichiometric formula is expanded to the more general form La0.3Sr0.7Fe1-xCrxO3(x=0, 0.1, 0.2 and 0.3), where Cr concentration is varied. The current work investigates by the use of density functional theory (DFT) method the effect of Cr stoichiometry on La0.3Sr0.7Fe1-xCrxO3 perovskite on the electronic properties, mechanical properties, and surface catalytic activity of CO2 reduction. Moreover, some calculations were carried out on SrCrO4 phase for comparing.

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ההרצאה תתקיים ביום חמישי , ה-19 בנובמבר 2020 בשעה 14:30
הסמינר יתקיים בזום
The lecture will take place on Thursday, November 19st 2020 at 14:30
Seminar by Zoom

https://zoom.us/j/98017532992