INTISARI

DESAIN KOMPUTASIONAL MATERIAL PADA KATALIS PtAg (111) *SURFACE* TERDOPING Au UNTUK PENGEMBANGAN *PROTON EXCHANGE MEMBRANE FUEL CELLS*

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Telah dilakukan penelitian berupa desain material katalis PtAg (111) *surface* terdoping Au untuk pengembangan *proton exchange membrane fuel cells* menggunakan metode komputasional berdasarkan *density functional theory*. Penelitian ini dilakukan dengan cara mengoptimasi struktur terdoping Au, perhitungan stabilitas energi, dan struktur elektronik geometri PtAg (111) *surface.* Hasil optimasi struktut posisi berupa struktur geometri material katalis PtAg (111) yang stabil dilihat dari gaya system partikel yang mendekati 0. Hasil dari perhitungan stabilitas energi menunjukkan bahwa penambahan Au pada PtAg (111) menurunkan energi ikat oksigen dengan nilai (E_b= -5,46 eV), lebih kecil daripada Pt (111) murni dan PtAg (111) dengan energi ikat (E_b= -5,53 eV dan E_b = -5,56 eV) sehingga dapat meningkatkan aktivitas katalis pada saat *oxygen reduction reaction*. Hasil perhitungan stabilitas energi juga menunjukkan bahwa penambahan doping Au pada PtAg (111) dapat mengubah energi segregrasi mendekati angka positif sebesar 0,2 eV yang menurunkan kemungkinan terpisahnya antara atom Pt dan Ag sehingga dapat meningkatkan durabilitas katalis pada saat *oxygen reduction reaction*. Hasil perhitungan struktur elektronik berupa pita elektronik yang menunjukkan PtAg (111) *surface* yang terdoping Au mempunyai sifat magnetik dan feroelektrik. Selain itu, dilihat dari *charge density* dan *density of state* menunjukkan terdapat adanya ikatan antara spesimen oksigen PtAg (111) *surface* terdoping Au.

Kata Kunci: PtAg (111) *surface* terdoping Au, *Density function theory* (DFT), *proton exchange membrane fuel cells* (PEMFC).

ABSTRACT

COMPUTATIONAL MATERIAL DESIGN OF Au DOPED PtAg (111) SURFACE CATALYST FOR DEVELOPMENT OF EXCHANGE MEMBRANE FUEL CELLS

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Research has been carried out in the form of surface Au-doped PtAg (111) catalyst material design for the development of proton exchange membrane fuel cells using a computational method based on density functional theory. This research was carried out by optimizing the Au-doped structure, calculating energy stability, and the electronic structure geometry of the PtAg (111) surface. The results of positional structure optimization are the geometric structure of the PtAg catalyst material (111) which is stable in terms of the particle system forces which are close to 0. The results of the energy stability calculations show that the addition of Au to PtAg (111) lowers the oxygen binding energy with a value of (Eb = -5.46 eV), which is smaller than pure Pt (111) and PtAg (111) with a binding energy (Eb = -5.53 eV and Eb = -5.56 eV) so that it can increase the activity of the catalyst during the oxygen reduction reaction. The results of energy stability calculations also show that the addition of Au doping to PtAg (111) can change the segregation energy to a positive number of 0.2 eV which reduces the possibility of separation between Pt and Ag atoms so as to increase the durability of the catalyst during the oxygen reduction reaction. The results of electronic structure calculations are in the form of electronic bands which show that the Au-doped PtAg (111) surface has magnetic and ferroelectric properties. In addition, the view of the charge density and density of state showed that there was a bond between the surface doped Au doped PtAg (111) oxygen specimens.

Keyword: PtAg (111) surface Au doped, Density function theory (DFT), proton exchange membrane fuel cells (PEMFC).