

Abstract Submitted
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Catalytic role of Au nanoparticle in GaAs nanowire growth¹ PETER KRATZER, SUNG SAKONG, VOLKER PANKOKE, University Duisburg-Essen, Germany — The energetics of Ga, As and GaAs species on the Au(111) surface (employed as a model for Au nanoparticles) is investigated by means of density-functional calculations. Apart from formation of the compound Au₇Ga₂, Ga is found to form a surface alloy with Au, with comparable $\Delta H \sim 0.5$ eV for both processes. Dissociative adsorption of As₂ is found to be exothermic by more than 2 eV on both clean Au(111) and AuGa surface alloys. The As-Ga species formed by reaction of As with the surface alloy is sufficiently stable to cover the surface of an Au particle *in vacuo* in contact with a GaAs substrate. Concerning the Au-catalysed growth of GaAs nanowires, we conclude that impingement of As₂ or As₄ molecules on the Au particle suffices as supply of arsenic to the growth zone. We identify a regime of temperatures and As₂ partial pressures suitable for Au-catalysed nanowire growth in molecular beam epitaxy.

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