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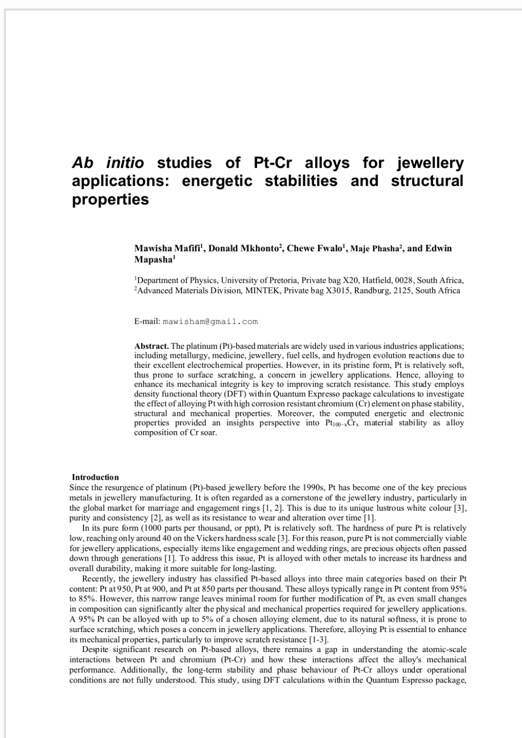

Ab initio studies of Pt-Cr alloys for jewellery applications: energetic stabilities and structural properties

Mawisha Mafifi[1], Donald Mkhonto[2], Chewe Fwalo[1], Maje Phasha[2], and Edwin Mapasha[1]

[1]Department of Physics, University of Pretoria, Private bag X20, Hatfield, 0028, South Africa,
[2]Advanced Materials Division, MINTEK, Private bag X3015, Randburg, 2125, South Africa

E-mail: mawisham@gmail.com

Abstract. The platinum (Pt)-based materials are widely used in various industries applications; including metallurgy, medicine, jewellery, fuel cells, and hydrogen evolution reactions due to their excellent electrochemical properties. However, in its pristine form, Pt is relatively soft, thus prone to surface scratching, a concern in jewellery applications. Hence, alloying to enhance its mechanical integrity is key to improving scratch resistance. This study employs density functional theory (DFT) within Quantum Expresso package calculations to investigate the effect of alloying Pt with high corrosion resistant chromium (Cr) element on phase stability, structural and mechanical properties. Moreover, the computed energetic and electronic properties provided an insights perspective into $Pt_{100-x}Cr_x$ material stability as alloy composition of Cr soar.

Introduction

Since the resurgence of platinum (Pt)-based jewellery before the 1990s, Pt has become one of the key precious metals in jewellery manufacturing. It is often regarded as a cornerstone of the jewellery industry, particularly in the global market for marriage and engagement rings [1, 2]. This is due to its unique lustrous white colour [3], purity and consistency [2], as well as its resistance to wear and alteration over time [1].

In its pure form (1000 parts per thousand, or ppt), Pt is relatively soft. The hardness of pure Pt is relatively low, reaching only around 40 on the Vickers hardness scale [3]. For this reason, pure Pt is not commercially viable for jewellery applications, especially items like engagement and wedding rings, are precious objects often passed down through generations [1]. To address this issue, Pt is alloyed with other metals to increase its hardness and overall durability, making it more suitable for long-lasting.

Recently, the jewellery industry has classified Pt-based alloys into three main categories based on their Pt content: Pt at 950, Pt at 900, and Pt at 850 parts per thousand. These alloys typically range in Pt content from 95% to 85%. However, this narrow range leaves minimal room for further modification of Pt, as even small changes in composition can significantly alter the physical and mechanical properties required for jewellery applications. A 95% Pt can be alloyed with up to 5% of a chosen alloying element, due to its natural softness, it is prone to surface scratching, which poses a concern in jewellery applications. Therefore, alloying Pt is essential to enhance its mechanical properties, particularly to improve scratch resistance [1-3].

Despite significant research on Pt-based alloys, there remains a gap in understanding the atomic-scale interactions between Pt and chromium (Pt-Cr) and how these interactions affect the alloy's mechanical performance. Additionally, the long-term stability and phase behaviour of Pt-Cr alloys under operational conditions are not fully understood. This study, using DFT calculations within the Quantum Espresso package,