

Abstract Submitted  
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**Thickness and surface-termination effects on magnetocrystalline anisotropy of FeM (M=Rh, Cr, and Pt) (001) thin films**<sup>1</sup> SOYOUNG JEKAL, SUNG-HYON RHIM, SOON-CHEOL HONG, Univ of Ulsan — FeM (M=Rh, Cr, and Pt) alloys show diverse interesting physical properties,<sup>2,3,4</sup> which attracted these alloys as a promising candidate for spintronics application.<sup>5</sup> In this study, we investigate effects of thickness and surface-termination on magnetism and magnetocrystalline anisotropies (MCAs) on the CsCl-structured FeM(001) thin films, using Vienna Ab initio Simulation Package. Two surface terminations (Fe-terminated and M-terminated) and thicknesses from 3 to 15 monolayers are taken into account. We find that magnetism and MCAs are sensitive to the surface termination and the thickness, whose relevance to electronic structures will be discussed.

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<sup>2</sup>X. Mart et al., *Nature Mater.* **13**, 367 (2014)

<sup>3</sup>S. L. Qiu, P. M. Marcus, and V. L. Moruzzi, *J. Appl. Phys.* **85**, 4839 (1999).

<sup>4</sup>G. Brown, B. Kraczek, A. Janotti, T. C. Schulthess, G. M. Stocks, and D. D. Johnson, *Phys. Rev. B* **68**, 052405 (2003).

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