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Electronic Structures of HfMoNbTaTiZr Alloy¹ SHIZHONG YANG,
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University and A&M College — Recent study shows HfMoNbTaTiZr alloy has
higher yield strength at 1200 degree C than HfMoTaTiZr alloy. To gain atomic level
understanding the mechanism, we studied the electronic structures of HfMoNbTa-
TiZr alloy from first principles density functional theory method and molecular
dynamics simulation. The results are compared with those of HfMoTaTiZr alloy.

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