# Electronic structure study of Fe-B alloy system

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We carried out first principle molecular dynamics simulation of iron based Fe-B alloy using Projector augmented wave method with in density functional theory to enquire electronic structure as well as to estimate glass forming ability, Simulations were conceded out in stable and undercooled state to get some structural information such as self diffusion coefficient, pair correlation function and to study the short range ordering for structural relaxation ,which may have repercussion to study the nature of glass forming ability.