博士論文公聴会の公示（物理学専攻）

学位申請者：　福市　真之

論文題目：First-Principles Calculations on the Origin of Mechanical Properties and Electronic Structures of 3*d*, 4*d*, and 5*d* Transition Metal Monocarbides
（3*d*，4*d*，5*d* 遷移金属炭化物の機械的性質と電子構造の起源に関する第一原理計算）

日時：2019 年 2 月 5 日（火） 16:20 — 17:50
場所：理学研究科 H 棟 7 階セミナー室（H701 号室）

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論文要旨：

Much is not systematically known about the origin of mechanical properties of 5*d* transition metal carbides including tungsten carbide applied as main materials of cutting instruments, dies, and other wear-resistant parts. To understand the microscopic origin of hardness in the carbides, the mechanical properties and electronic structures of 5*d* transition metal monocarbides *M*C (*M* = Hf, Ta, W, Re, Os, Ir, and Pt) in five different crystal structures (NaCl, WC, ZnS, CsCl, and NiAs-type structures) are analyzed using first-principles density-functional-theory calculations. Our results indicate that WC-type WC and NiAs-type ReC have the highest and second highest hardness among all of the *M*C, respectively. It is found that *M*C in the ranges of less than and more than half filled 5*d* shells are brittle and ductile, respectively and filling in the bonding and anti-bonding states contributes to brittleness and ductility. The Debye temperature could be a key to understanding the origin of hardness in terms of bulk and shear moduli. The microscopic mechanisms of hardness and brittleness in 3*d*, 4*d*, and 5*d* transition metal monocarbides are discussed in detail.