Materials Design by Computer Simulation 2001

Mizuseki, H; Jin, Y; Kawazoe, Y; Wille, LT

Cluster growth processes by direct simulation Monte Carlo method

Appl. Phys. A-Mater. Sci. Process. 73 (2001) 731 – 735

01-IMR0189

Wang, JT; Wang, DS; Kawazoe, Y

Magnetic phase competing in MnAu systems

Appl. Phys. Lett. 79 (2001) 1507 – 1509

01-IMR0190

Jeong, GH; Hatakeyama, R; Hirata, T; Tohji, K; Motomiya, K; Sato, N; Kawazoe, Y

Structural deformation of single-walled carbon nanotubes and fullerene encapsulation due to magnetized-plasma ion irradiation

Appl. Phys. Lett. 79 (2001) 4213 – 4215

01-IMR0191

Zhou, G; Kawazoe, Y

Application of single-walled carbon nanotube body to unique emitter: a first-principles study

Chem. Phys. Lett. 350 (2001) 386 – 392

01-IMR0192

Guo, Y; Wang, B; Gu, BL; Kawazoe, Y

Asymmetry and separation of spin tunneling time in ZnSe/Zn1-xMnxSe multilayers

Eur. Phys. J. B 23 (2001) 509 – 513

01-IMR0193

Esfarjani, K; Farajian, AA; Ebrahimi, F; Kawazoe, Y

Transport properties of a nanotube-based transistor

Eur. Phys. J. D 16 (2001) 353 – 355

01-IMR0194

Zeng, Z; Mizuseki, H; Simamura, K; Fukuda, T; Higashino, K; Kawazoe, Y

Three-dimensional oscillatory thermocapillary convection in liquid bridge under microgravity

Int. J. Heat Mass Transf. 44 (2001) 3765 – 3774

01-IMR0195

Parlinski, K; Kawazoe, Y; Waseda, Y

Ab initio studies of phonons in CaTiO3

J. Chem. Phys. 114 (2001) 2395 – 2400

01-IMR0196

Zeng, Z; Mizuseki, H; Shimamura, K; Higashino, K; Fukuda, T; Kawazoe, Y

Marangoni convection in model of floating zone under microgravity

J. Cryst. Growth 229 (2001) 601 – 604

01-IMR0197

Sahara, R; Mizuseki, H; Ohno, K; Kubo, H; Kawazoe, Y

Lattice Monte Carlo simulation with a renormalized potential in Si

J. Cryst. Growth 229 (2001) 610 – 614

01-IMR0198

Wang, JT; Zhou, L; Wang, DS; Kawazoe, Y

Exchange interaction and magnetic phase transition in layered Fe/Au superlattices

J. Magn. Magn. Mater. 226 (2001) 633 – 634

01-IMR0199

Kawazoe, Y; Ohno, K; Esfarjani, K; Maruyama, Y; Shiga, K; Farajian, A

Why the all-electron full-potential approach is suitable for calculations on fullerenes and nanotubes?

J. Mol. Graph. 19 (2001) 270 – 273

01-IMR0200

Yu, JZ; Sun, Q; Wang, Q; Kawazoe, Y

Magnetic phase transition and hydrogen solubility in Fe, Co, and Ni

J. Phase Equilib. 22 (2001) 504 – 507

01-IMR0201

Majumder, C; Mizuseki, H; Kawazoe, Y

Molecular scale rectifier: Theoretical study

J. Phys. Chem. A 105 (2001) 9454 – 9459

01-IMR0202

Sun, Q; Wang, Q; Yu, JZ; Ohno, G; Kawazoe, Y

First-principles studies on pure and doped C-32 clusters

J. Phys.-Condes. Matter 13 (2001) 1931 – 1938

01-IMR0204

Katayama-Yoshida, H; Nishimatsu, T; Yamamoto, T; Orita, N

Codoping method for the fabrication of low-resistivity wide band-gap semiconductors in p-type GaN, p-type AlN and n-type diamond: prediction versus experiment

J. Phys.-Condes. Matter 13 (2001) 8901 – 8914

01-IMR0206

Berne, C; Sluiter, M; Kawazoe, Y; Pasturel, A

Ordering effects in the Re-W and Re-Ta sigma phases

J. Phys.-Condes. Matter 13 (2001) 9433 – 9443

01-IMR0207

Taneda, A; Shimizu, T; Kawazoe, Y

Stable disordered structures of vanadium clusters

J. Phys.-Condes. Matter 13 (2001) L305 – L312

01-IMR0205

Chui, ST; Wang, JT; Zhou, L; Esfarjani, K; Kawazoe, Y

Realization of an effective ultrahigh magnetic field on a nanoscale

J. Phys.-Condes. Matter 13 (2001) L49 – L55

01-IMR0203

Shishido, T; Kudou, K; Okada, S; Ye, JH; Yoshikawa, A; Sasaki, T; Oku, M; Horiuchi, H; Higashi, I; Kohiki, S; Kawazoe, Y; Nakajima, K

R-dependency of the hardness of perovskite-type RRh3B compounds (R = La, Gd, Lu and Sc)

Jpn. J. Appl. Phys. Part 1 – Regul. Pap. Short Notes Rev. Pap. 40 (2001) 6037 – 6038

01-IMR0039

Kawazoe, Y

How well can physical, chemical, and mechanical properties of materials be predicted by ab initio techniques?

Mater. Des. 22 (2001) 61 – 67

01-IMR0208

Kawazoe, Y; Kohyama, M

Special issue on advances in computational materials science and engineering II – Preface

Mater. Trans. 42 (2001) 2149 – 2149

01-IMR0214

Ishii, S; Ohno, K; Kawazoe, Y

Comparison between the full frequency integration and the GPP model in ab-initio GW calculation of Na clusters

Mater. Trans. 42 (2001) 2150 – 2152

01-IMR0215

Wang, Q; Sun, Q; Briere, TM; Kawazoe, Y

First-principles study of the magic Ar6Fe+ cluster

Mater. Trans. 42 (2001) 2172 – 2174

01-IMR0216

Kawamura, H; Kumar, V; Sun, Q; Kawazoe, Y

Bonding character of hydrogen in aluminum clusters

Mater. Trans. 42 (2001) 2175 – 2179

01-IMR0217

Belosludov, RV; Takami, S; Kubo, M; Miyamoto, A; Kawazoe, Y

Theoretical study on Fe-based metal clusters: Application in heterogeneous catalysis

Mater. Trans. 42 (2001) 2180 – 2183

01-IMR0218

Shiga, K; Ohno, K; Ohtsuki, T; Kawazoe, Y

Formation of N-doped C-60 studied by ab initio molecular dynamics simulations

Mater. Trans. 42 (2001) 2189 – 2193

01-IMR0219

Belosludov, VR; Inerbaev, TM; Luzhkovskaya, ND; Kawazoe, Y

Elastic moduli and absolute stability limits of clathrate hydrates of structure I at positive and negative pressures

Mater. Trans. 42 (2001) 2194 – 2200

01-IMR0220

Sluiter, MHF; Kawazoe, Y

Bondlengths and phase stability of Silicon-Germanium alloys under pressure

Mater. Trans. 42 (2001) 2201 – 2205

01-IMR0221

Lu, JQ; Chen, H; Wu, J; Mizuseki, H; Kawazoe, Y

Ab initio modeling of real molecular logic devices

Mater. Trans. 42 (2001) 2270 – 2275

01-IMR0222

Majumder, C; Mizuseki, H; Kawazoe, Y

Bipyridinium molecular switch: Ab-initio electronic structure calculation

Mater. Trans. 42 (2001) 2276 – 2278

01-IMR0223

Vannarat, S; Esfarjani, K; Chui, ST; Kawazoe, Y

Effect of elastic interaction on self-assembled island spatial arrangement

Mater. Trans. 42 (2001) 2279 – 2282

01-IMR0224

Jin, Y; Mizuseki, H; Kawazoe, Y

Direct Simulation Monte Carlo for cluster growth process in rarefied gas

Mater. Trans. 42 (2001) 2295 – 2298

01-IMR0225

Zeng, Z; Mizuseki, H; Higashino, K; Shimamura, K; Fukuda, T; Kawazoe, Y

Structure similarity of mixed buoyancy-thermocapillary flow in half-zone liquid bridge

Mater. Trans. 42 (2001) 2322 – 2331

01-IMR0226

Wang, HP; Sluiter, M; Kawazoe, Y

Interfacial segregation of early transition metals in nickel aluminide

Mater. Trans. 42 (2001) 407 – 410

01-IMR0209

Aihara, T; Kaneko, R; Sluiter, MHF; Kawazoe, Y

Molecular dynamics simulation of temperature dependence of dislocation behavior in fcc Ni single crystal under tensile condition

Mater. Trans. 42 (2001) 425 – 428

01-IMR0210

Vannarat, S; Sluiter, MHF; Kawazoe, Y

Strain dependence of solute atom energy in aluminum-rich alloys

Mater. Trans. 42 (2001) 429 – 431

01-IMR0211

Bae, YC; Osanai, H; Ohno, K; Sluiter, M; Kawazoe, Y

All-electron mixed-basis calculation to optimize structures of vanadium clusters

Mater. Trans. 42 (2001) 432 – 434

01-IMR0212

Hongo, K; Mizuseki, H; Kawazoe, Y

A Monte Carlo simulation on the process of cluster deposition

Mater. Trans. 42 (2001) 439 – 442

01-IMR0213

Taghavinia, N; Lerondel, G; Makino, H; Yamamoto, A; Yao, T; Kawazoe, Y; Goto, T

Nanocrystalline Zn2SiO4 : Mn2+ grown in oxidized porous silicon

Nanotechnology 12 (2001) 547 – 551

01-IMR0227

Guo, Y; Lu, JQ; Zeng, Z; Wang, Q; Gu, BL; Kawazoe, Y

Quantum size effect and temperature effect on spin-polarized transport in ZnSe/Zn1-xMnxSe multilayers

Phys. Lett. A 284 (2001) 205 – 215

01-IMR0228

Guo, Y; Wang, B; Gu, BL; Kawazoe, Y

Spin-tunneling time in a hybrid semimagnetic/semiconductor heterostructure with a single paramagnetic layer

Phys. Lett. A 291 (2001) 453 – 458

01-IMR0229

Sun, Q; Wang, Q; Yu, JZ; Briere, TM; Kawazoe, Y

Structure and interaction mechanism in the magic Al13+H2O cluster

Phys. Rev. A 64 (2001) Art. No. 053203 –

01-IMR0230

Kumar, V; Kawazoe, Y

Evolution of electronic states and abnormal multishell relaxations in strontium clusters

Phys. Rev. B 63 (2001) Art. No. 075410 –

01-IMR0231

Yoshihara, A; Wang, JT; Takanashi, K; Himi, K; Kawazoe, Y; Fujimori, H; Grunberg, P

Interlayer exchange coupling in fine-layered Fe/Au superlattices

Phys. Rev. B 63 (2001) Art. No. 100405 –

01-IMR0232

Ishii, S; Ohno, K; Kawazoe, Y; Louie, SG

Ab initio GW quasiparticle energies of small sodium clusters by an all-electron mixed-basis approach

Phys. Rev. B 63 (2001) Art. No. 155104 –

01-IMR0233

Sun, Q; Wang, Q; Yu, JZ; Kumar, V; Kawazoe, Y

Real-space representation of electron localization and shell structure in jelliumlike clusters

Phys. Rev. B 63 (2001) Art. No. 193408 –

01-IMR0234

Guo, Y; Gu, BL; Wang, H; Kawazoe, Y

Spin-resonant suppression and enhancement in ZnSe/Zn1-xMnxSe multilayer heterostructures

Phys. Rev. B 63 (2001) Art. No. 214415 –

01-IMR0235

Suzuki, T; Hasegawa, Y; Li, ZQ; Ohno, K; Kawazoe, Y; Sakurai, T

Electron standing-wave observation in the Pd overlayer on Au(111) and Cu(111) surfaces by scanning tunneling microscopy

Phys. Rev. B 64 (2001) Art. No. 081403 –

01-IMR0103

Kumar, V; Kawazoe, Y

Hund's rule in metal clusters: Prediction of high magnetic moment state of Al12Cu from first-principles calculations

Phys. Rev. B 64 (2001) Art. No. 115405 –

01-IMR0237

Ohtsuki, T; Ohno, K; Shiga, K; Kawazoe, Y; Maruyama, Y; Shikano, K; Masumoto, K

Formation of Sb- and Te-doped fullerenes by using nuclear recoil and molecular-dynamics simulations

Phys. Rev. B 64 (2001) Art. No. 125402 -

01-IMR0238

Berne, C; Sluiter, M; Kawazoe, Y; Hansen, T; Pasture, A

Site occupancy in the Re-W sigma phase

Phys. Rev. B 64 (2001) Art. No. 144103 -

01-IMR0239

Guo, Y; Lu, JQ; Gu, BL; Kawazoe, Y

Spin-resonant splitting in magnetically modulated semimagnetic semiconductor superlattices

Phys. Rev. B 64 (2001) Art. No. 155312 -

01-IMR0240

Vannarat, S; Sluiter, MHF; Kawazoe, Y

First-principles study of solute-dislocation interaction in aluminum-rich alloys

Phys. Rev. B 64 (2001) Art. No. 224203 -

01-IMR0241

Majumder, C; Kumar, V; Mizuseki, H; Kawazoe, Y

Small clusters of tin: Atomic structures, energetics, and fragmentation behavior

Phys. Rev. B 64 (2001) Art. No. 233405 -

01-IMR0242

Yamamoto, A; Syouji, A; Goto, T; Kulatov, E; Ohno, K; Kawazoe, Y; Uchida, K; Miura, N

Excitons and band structure of highly anisotropic GaTe single-crystals

Phys. Rev. B 64 (2001) Art. No.035210 -

01-IMR0236

Kumar, V; Kawazoe, Y

Metal-encapsulated fullerenelike and cubic caged clusters of silicon

Phys. Rev. Lett. 87 (2001) Art. No. 045503 -

01-IMR0243

Nishimatsu, T; Katayama-Yoshida, H; Orita, N

Theoretical study of hydrogen-related complexes in diamond for low-resistive n-type diamond semiconductor

Physica B 302 (2001) 149 - 154

01-IMR0244

Ohtsuki, T; Ohno, K; Shiga, K; Kawazoe, Y; Maruyama, T; Shikano, K; Masumoto, K

Formation of new materials in fullerene by using nuclear recoil: Antimony case

Scr. Mater. 44 (2001) 1575 - 1578

01-IMR0245

Ohno, K; Kawazoe, Y

Abnormal intermolecular interaction between overlayer C-60 molecules due to induced dipole moments in C-60 thin films adsorbed on substrates

Scr. Mater. 44 (2001) 1579 - 1582

01-IMR0246

Mizuseki, H; Hongo, K; Kawazoe, Y; Wille, LT

Multiscale simulation of cluster growth and deposition processes by direct simulation Monte Carlo method

Scr. Mater. 44 (2001) 1911 – 1914

01-IMR0247

Kumar, V; Kawazoe, Y

Icosahedral growth and non-metal-metal transition in strontium clusters

Scr. Mater. 44 (2001) 1949 – 1953

01-IMR0248

Wang, Q; Sun, Q; Yu, ZJ; Sakurai, M; Kawazoe, Y

Capacitance of magic Ba-n clusters

Scr. Mater. 44 (2001) 1959 – 1962

01-IMR0249

Ishii, S; Ohno, K; Kawazoe, Y

Ab-initio quasiparticle energies of small sodium clusters by the GW approximation

Scr. Mater. 44 (2001) 1963 – 1966

01-IMR0250

Wang, Q; Sun, Q; Yu, JZ; Kawazoe, Y

Nonmetal-metal transition in Ba-n clusters

Solid State Commun. 117 (2001) 635 – 639

01-IMR0251
