ABD1: MHC Class I A*0201-LLFGYPVYV-A6 TCR complex

Convergence diagnostics of number density

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Keywords: Quantum Immunology, Major Histocompatibility Complex (MHC), peptide (p), T Cell Receptor (TCR), Molecular Dynamics (MD), Competing Mode Decomposition (CMD).

A. Study scope Quantum Immunology ¹⁻¹⁵ Protein short-range order (SRO) ¹⁶⁻³²	B. Methods Molecular dynamics Parameter set: CHARMM22 Water model: TIP3P Solvent padding: 40 Å Periodic boundary conditions: Yes MD Ensemble: Isothermal–isobaric (NPT) Room temperature (RT): 25 °C Physiological temperature (PT): 37 °C Convergence diagnostics Competing Mode Decomposition
C. pMHC-TCR complex details MHC type: A*0201 (Homo sapiens) MHC sequence GSHSMRYFFTSVSRPGRGEPRFIAVG YVDDTQFVRFDSDAASQRMEPRAPWIEQEGPEYWDGETR KVKAHSQTHRVDLGT LRGYYNQSEAGSHTVQRM YGCDVGSDWRFLRGYHQYAYDGKD YIALKEDLRSWTAADMAAQ TTKHKWEAAHVAEQ LRAYLEG TCVEWLRRLRYL ENGKETLQRTDAPKTHMTHHAVSDHEATLR CWALSFYPAEITLTWQRDGEDQTQDTELVETRPAGDGT FQK WAAVVVPSGQEQRYTCHVQHEGLPKPLTLRWE MHC mutations: None Peptide gene/comments TAX protein of human T-lymphotropic virus type 1 Peptide sequence LLFGYPVYV TCR type: A6 (Homo sapiens) TCR-α sequence KEVEQNSGPLSVPEGAIASLNCTYS DRGSQSFFWYRQYSGKSP ELIMSIYSNGDKEDGRFTAQLNKASQYV SLLIRDSQPS DSATYLC AVTTDSWGKLQFGAGTQVVVTPDIQNPDP AVYQLRDSKSSDKSVCLFTDFDSQTNVSQSKSDVYITDKTVLDM RSMDFKNSA VAWSNKSDFACANAFNNSIIPEDTFFPSP ESS TCR-α mutations: None TCR-β sequence NAGVTQTPKFQVLK TGQSM TLQCAQDMNHEYMSWYRQDPGMGLRLIHY SVGAGITDQGEVPNGYNVSRSTEDFPLRLLSA APSQTSVYFCASR PGLAGGRPEQYFGPGTRLTVTEDLKNVFPPEVAVFEPSEAEISHTQKATLVCLATGFYPDHVELS WVV NGKEVHSGVSTDPQPLKEQPALNDSRYALSSRLRVSATFWQNPRNHFR CQVQFYGLSENDEWTQDRAKPVTQIVSAEAWGR AD TCR-β mutations: None

Figure 1. ABD1 supercell number density, ρ , vs. MD time for (a) RT and (d) PT. CMD convergence analysis of ρ vs. MD time for (b) RT and (e) PT. (c) Probability density function of the RT ρ trajectory (Fig.1a), blue bars, and of the RT ρ sample means (sample size of 30), yellow bars. (f) Probability density function of the PT ρ trajectory (Fig.1d), blue bars, and of the PT ρ sample means (sample size of 30), yellow bars. See Table 1 for convergence diagnostics.

Table 1. Convergence diagnostics.

Temperature: RT

Time (ns): 99.6

Type: partial

Residual time for full convergence (ns): 21.7

Temperature: PT

Time (ns): 78.7

Type: partial

Residual time for full convergence (ns): 30.4

Conflict of interest

It is declared that there is no conflict of interest.

Author contributions

Analysis was based on precursor theoretical modelling related to atomic and mesoscale systems^{1-13,16-60}.

References

- 1 Germenis, A. E., Manousakis, M. N. & Antipas, G. S. E. The Dawn of Quantum Immunology. *SRL Immunology and Immunotherapy* **1**, 3-6 (2016).
- 2 Antipas, G. S. E. & Germenis, A. E. Atomic coordination reflects peptide immunogenicity. *Frontiers in Molecular Biosciences* **2**, doi:10.3389/fmolb.2015.00077 (2016).
- 3 Antipas, G. S. E. & Germenis, A. E. The coordination of unprotonated peptide tertiary structure as a metric of pMHC–TCR functional avidity. *Data In Brief* **5**, 342-347, doi:10.1016/j.dib.2015.09.009 (2015).
- 4 Antipas, G. S. E. & Germenis, A. E. Human Cytomegalovirus variant peptides adapt by decreasing their total coordination upon binding to a T cell receptor. *Data In Brief* **4**, 492-499, doi:10.1016/j.dib.2015.07.019 (2015).
- 5 Antipas, G. S. E. & Germenis, A. E. The quantum chemical causality of pMHC-TCR biological avidity: peptide atomic coordination data and the electronic state of agonist N termini. *Data In Brief* **3**, 180-184, doi:10.1016/j.dib.2015.02.021 (2015).
- 6 Antipas, G. S. E. & Germenis, A. E. Quantum chemical calculations predict biological function: The case of T cell receptor interaction with a peptide/MHC class I. *Frontiers in Chemistry* **3**, doi:10.3389/fchem.2015.00009 (2015).
- 7 Antipas, G. S. E. & Germenis, A. E. in *IUPHAR Immunopharmacology Section - 8th Biannual Meeting of the Hellenic Society of Basic & Clinical Pharmacology* (Athens, Greece, 2014).
- 8 Karalis, K., Karalis, N., Karkalos, N., Antipas, G. & Xenidis, A. Computational fluid dynamics analysis of a three-dimensional electric submerged arc furnace operation. *OSF Preprints*, doi:10.31219/osf.io/xgnse (2020).
- 9 Antipas, G. S. E., Ntallis, N. A. & Karalis, K. T. MHC Class I H-2Kb-INFDFNTI-BM3.3 TCR complex: Convergence diagnostics of internal energy and density. *OSF Preprints*, doi:10.31219/osf.io/tp78g (2020).
- 10 Antipas, G. S. E., Ntallis, N. A. & Karalis, K. T. MHC Class I A*0201-LLFGYPVYV-B7 TCR complex: Convergence diagnostics of internal energy and density. *OSF Preprints*, doi:10.31219/osf.io/yzces (2020).
- 11 Antipas, G. S. E., Ntallis, N. A. & Karalis, K. T. MHC Class I A*0201-LLFGYAVYV-A6 TCR complex: Convergence diagnostics of internal energy and density. *OSF Preprints*, doi:10.31219/osf.io/h5a32 (2020).
- 12 Antipas, G. S. E., Ntallis, N. A. & Karalis, K. T. MHC Class I A*0201-LLFGYPRYV-A6 TCR complex: Convergence diagnostics of internal energy and density. *OSF Preprints*, doi:10.31219/osf.io/tjxzw (2020).
- 13 Antipas, G. S. E., Ntallis, N. A. & Karalis, K. T. MHC Class I A*0201-LLFGYPVYV-A6 TCR complex: Convergence diagnostics of internal energy and density. *OSF Preprints*, doi:10.31219/osf.io/sgwr5 (2020).
- 14 Antipas, G. S. E. & Ntallis, N. A. MHC Class I H-2Kb-SIYRYGL-2C TCR complex: convergence diagnostics of number density. *OSF Preprints*, doi:10.31219/osf.io/3xn5m (2020).
- 15 Antipas, G. S. E. & Ntallis, N. A. MHC Class I H-2Kb-SIYRYGL-2C TCR complex: convergence diagnostics of internal energy. *OSF Preprints*, doi:10.31219/osf.io/fudre (2020).
- 16 Antipas, G. S. E. & Ntallis, N. A. Relaxation Time-Approximation method for the efficient detection of critical states in reactive trajectories. *OSF Preprints*, doi:10.31219/osf.io/8vnm7 (2020).

- 17 Antipas, G. S. E. & Karalis, K. T. Direct determination of amorphous number density from the reduced pair distribution function. *MethodsX* **6**, 601-605, doi:10.1016/j.mex.2019.03.005 (2019).
- 18 Karalis, K. T., Dellis, D., Antipas, G. S. E. & Xenidis, A. Bona-fide method for the determination of short range order and transport properties in a ferro-aluminosilicate slag. *Scientific reports* **6**, 30216, doi:10.1038/srep30216 (2016).
- 19 Antipas, G. S. E., Mangiorou, E. & Hristoforou, E. The effect of Indium content on the atomic environment and cluster stability of $\text{GeSe}_4\text{In}_{x=10,15}$ metallic glasses. *Metals* **5**, 102-118, doi:10.3390/met5010102 (2015).
- 20 Antipas, G. S. E. Formation energies associated to the growth, inter-diffusion and surface alloying of Cr and Nb single layers on a pure Cu substrate. *Annals of Materials Research* (2015).
- 21 Antipas, G. S. E. A concise methodology for the estimation of elemental concentration effects on mesoscale cohesion of non-ferrous covalent glasses: the case of $\text{Se}_{(80-x)}\text{Ge}_{(20-x)}\text{In}_{x=0,5,10,15}$. *Data In Brief* **4**, 257-265, doi:10.1016/j.dib.2015.05.024 (2015).
- 22 Statharas, E., Tserotas, P. & Antipas, G. S. E. Experimental and First Principles' Characterization of Functionalized Magnetic Nanoparticles. *Key Engineering Materials* **605**, 681-684, doi:10.4028/www.scientific.net/KEM.605.681 (2014).
- 23 Karalis, K., Temleitner, L., Antipas, G. S. E., Pusztai, L. & Xenidis, A. Experimentally constrained atomic order probing of a Si-Al composite glass. *Philosophical Magazine*, 1-9, doi:10.1080/14786435.2013.863438 (2014).
- 24 Antipas, G. S. E., Papassiopi, N. & Xenidis, A. On the elusive anti-bayerite structure. *Solid State Ionics* **255**, 65-73, doi:10.1016/j.ssi.2013.11.052 (2014).
- 25 Antipas, G. S. E., Mangiorou, E. & Hristoforou, E. Solute-solvent interactions and atomic cohesion in GeSe_4 and GeSe_4In_5 metallic glasses. *Materials Research Express* **1**, 015202, doi:10.1088/2053-1591/1/1/015202 (2014).
- 26 Antipas, G. S. E. & Mangiorou, E. Atomic topology and electronic structure of a melt-spun Al_{92}U_8 metallic glass. *Computational and Theoretical Chemistry* **1036**, 16-21, doi:10.1016/j.comptc.2014.03.009 (2014).
- 27 Antipas, G. S. E. & Karalis, K. The effect of annealing on the electronic stability of an amorphous $\text{Zr}_{70}\text{Pd}_{30}$ alloy. *Materials Chemistry and Physics* **147**, 1092-1098, doi:10.1016/j.matchemphys.2014.06.063 (2014).
- 28 Antipas, G. S. E. Short range order and stability of a mechanically alloyed $\text{Cr}_{25}\text{Nb}_{75}$ alloy determined by total scattering and first principles. *Materials Research* **17**, 1677-1685, doi:10.1590/1516-1439.323014 (2014).
- 29 Antipas, G. S. E., Temleitner, L., Karalis, K., Pusztai, L. & Xenidis, A. Atomic order and cluster energetics of a 17 w.t.% Si-based glass versus the liquid phase. *Journal of Physics: Condensed Matter* **25**, 1-7, doi:10.1088/0953-8984/25/45/454206 (2013).
- 30 Antipas, G. S. E., Statharas, E., Tserotas, P., Papadopoulos, N. & Hristoforou, E. Experimental and First-Principles Characterization of Functionalized Magnetic Nanoparticles. *ChemPhysChem* **14**, 1934-1942, doi:10.1002/cphc.201300161 (2013).
- 31 Antipas, G. S. E. Molecular orbital interactions in glass-forming $\text{Zr}_{70}\text{Cu}_{30}$ liquid quasicrystals. *Journal of Alloys and Compounds* **578**, 565-570, doi:10.1016/j.jallcom.2013.06.179 (2013).
- 32 Antipas, G. S. E. *et al.* A containerless study of short-range order in high-temperature Fe–Si–Al–Ca–Mg–Cr–Cu–Ni oxide systems. *Journal of Molecular Structure* **1019**, 151-158, doi:10.1016/j.molstruc.2012.03.056 (2012).
- 33 Antipas, G. S. E. & Karalis, K. T. Direct determination of amorphous number density from the reduced Pair Distribution Function. *OSF Preprints*, doi:10.31219/osf.io/n7gk9 (2020).
- 34 Karalis, K., Karkalos, N., Antipas, G. S. E. & Xenidis, A. Pragmatic analysis of the EAF continuum. *Royal Society Open Science*, doi:10.1098/rsos.170313 (2017).
- 35 Karalis, K. *et al.* A CFD analysis of slag properties, electrode shape and immersion depth effects on electric submerged arc furnace heating in ferronickel processing. *Applied Mathematical Modelling*, doi:10.1016/j.apm.2016.05.045 (2016).
- 36 Karalis, K., Karkalos, N., Antipas, G. S. E. & Xenidis, A. in *Metal 2015*.
- 37 Antipas, G. S. E. Improvement of the micro-hardness and wear resistance of various light alloys by plasma-sensitization. *Annals of Materials Research* (2015).

- 38 Antipas, G. S. E. Plasma-driven mechanisms of the surface modification of an Al6061 alloy. *Annals of Materials Research* (2015).
- 39 Antipas, G. S. E. Experimental and first principles assessment of plasma attenuation during laser treatment of an Al alloy. *Transactions of the IMF* **93**, 53-56, doi:10.1179/0020296714Z.000000000226 (2015).
- 40 Antipas, G. S. E. Superlattice-ordered PtPb intermetallics for environmental applications. *Annals of Materials Research* (2015).
- 41 Papassiopi, N. *et al.* A XAFS study of plain and composite iron(III) and chromium(III) hydroxides. *Chemosphere* **111**, 169-176, doi:10.1016/j.chemosphere.2014.03.059 (2014).
- 42 Antipas, G. S. E. & Statharas, E. Surface properties of a laser-irradiated Al 6061 alloy. *International Journal of Computational Materials Science and Surface Engineering* **6**, 1-12, doi:10.1504/IJCMSSE.2014.063755 (2014).
- 43 Antipas, G. S. E. Mechanical properties of a particle-reinforced Zr bulk metallic glass. *International Journal of Materials* **1**, 149-151 (2014).
- 44 Antipas, G. S. E. Plasma-spray synthesis and characterization of Ti-based nitride and oxide nanogranules. *Materials Research*, 0-0, doi:10.1590/1516-1439.252013 (2014).
- 45 Antipas, G. S. E. Surface growth and diffusion energetics of Ag monolayers on Cu (001). *Metals* **4**, 108-117, doi:10.3390/met4020108 (2014).
- 46 Antipas, G. S. E. Augmentation of wear-protective coatings for non-ferrous alloys by the addition of Cr and Ni elements. *Materials Research*, doi:10.1590/1516-1439.211013 (2014).
- 47 Antipas, G. S. E. A mass efficiency test of α - β processed Ti-Al-V alloys. *Key Engineering Materials* **605**, 605-608, doi:10.4028/www.scientific.net/KEM.605.605 (2014).
- 48 Papassiopi, N., Vaxevanidou, K., Christou, C., Karagianni, E. & Antipas, G. S. E. Synthesis, characterization and stability of Cr(III) and Fe(III) hydroxides. *Journal of hazardous materials*, doi:10.1016/j.jhazmat.2013.09.058 (2013).
- 49 Antipas, G. S. E. The Effect of Increasing Sn Content on High-Temperature Mechanical Deformation of an Mg-3%Cu-1%Ca Alloy. *Metals* **3**, 337-342, doi:10.3390/met3040337 (2013).
- 50 Antipas, G. S. E. Review of gas atomization and spray forming phenomenology. *Powder Metallurgy*, doi:10.1179/1743290113Y.00000000057 (2013).
- 51 Antipas, G. S. E. *et al.* in *RMC5* (Budapest, Hungary, 2012).
- 52 Antipas, G. S. E. Spray forming of al alloys: Experiment and theory. *Materials Research* **15**, 131-135, doi:10.1590/S1516-14392012005000007 (2012).
- 53 Antipas, G. Gas Atomization of Aluminium Melts: Comparison of Analytical Models. *Metals* **2**, 202-210, doi:10.3390/met2020202 (2012).
- 54 Antipas, G. S. E., Lekakou, C. & Tsakiroopoulos, P. Microstructural characterisation of Al—Hf and Al—Li—Hf spray deposits. *Materials Characterization* **62**, 402-408, doi:10.1016/j.matchar.2011.02.001 (2011).
- 55 Antipas, G. S. E. Liquid column deformation and particle size distribution in gas atomisation. *International Journal of Computational Materials Science and Surface Engineering* **4**, 247-264, doi:10.1504/IJCMSSE.2011.042822 (2011).
- 56 Antipas, G. S. E. Modelling of the break up mechanism in gas atomization of liquid metals Part II. The gas flow model. *Computational Materials Science* **46**, 955-959, doi:10.1016/j.commatsci.2009.04.046 (2009).
- 57 Antipas, G. S. E. Modelling of the break up mechanism in gas atomization of liquid metals. Part I: The surface wave formation model. *Computational Materials Science* **35**, 416-422, doi:10.1016/j.commatsci.2005.03.009 (2006).
- 58 Antipas, G. S. E. *Mathematical modeling of metal spray forming*. (original manuscript Oxford, 1998. Published as eBook, National Library of Greece) ISBN 978-618-80686-1-2, 1998).
- 59 Hunt, J. D., Antipas, G. & Thomas, R. W. *Alloy: solidification modeling*. (1996).
- 60 Antipas, G., Lekakou, C. & Tsakiroopoulos, P. The break up of melt streams by high pressure gases in spray forming. *Proceedings of the Second International Conference on Spray Forming*, 15-24 (1993).