Response to Reviewer 1 Comments

Point 1: In introduction, the use of 6000 series Al–Mg–Si alloys for manufacturing automobile body panels 24 has increased because such alloys exhibit hardening characteristics. The authors should be give the detailed reference cites.

Response 1: We thank the reviewer for this suggestion. We have added references [1-6] about hardening characteristics in Al-Mg-Si alloys.

Point 2: In the last of page 2, a proper explanation should be provided to interpret why the length of the Si–Si bond in the β″-eye is longer than that in the layered VMg4Si8 complex.

Response 2: In the β″-eye, to accommodate the Mg-Si bonds in the Si layers, the Si-Si bonds are expanded. We have added a sentence to explain the length of the Si-Si bond.

Point 3: In methods section, “To examine the reproduction of the vacancy–solute complexes from the solid solution in the Al–Mg–Si alloy, we performed the first-principles-based MC simulations at 200 K”. The authors why choose simulations at 200 K? rather than others like 300 K.

Response 3: To avoid an excessive increase in the potential energy, we employed 200 K for the MC simulations. We have added Appendix A to explain why we employed 200 K for the MC simulations.

Point 4: In page 4, to illustrate the bonding between atoms, the authors should give detailed mechanism pictures, e.g., explaining the number of bonds between Mg-Si by charge density.

Response 4: We thank the reviewer for this suggestion. Considering the reviewer's suggestion, to evaluate the change in the stability of the β″-eye with increasing Mg atoms, we have calculated the formation energies of the layered $V\mathrm{Mg_4Si_8}+\mathrm{Mg}_n$ (n = 1–5) complexes with the β″-eye arrangement and the results are shown in Fig.6. We have added sentences about the change in the stability of the β″-eye in Lines: 152-161.

Point 5: In page 4, “There is a steep drop both in the formation energy and the binding energy of the VMg4Si8+Mg5 complex.” the authors need to mention the reason for the steepness.

Response 5: The reason for the steep drop was written in Lines:135-140 in the original manuscript (Lines:141-146 in the revised manuscript) as follows: “The steep decrease in the formation and binding energies of the $V\mathrm{Mg_4Si_8}+\mathrm{Mg_5}$ complex arises from not only the formation of Mg–Si bonds but also the

weakening of the repulsive Mg–Mg interaction."

Point 6: In page 5, Figure 5 shows the average lengths of the Mg–Si, Si–Si, and Mg–Mg bonds... The average length of the Mg–Si bond remains almost constant at 2.80 Å, which are obvious larger than those of Si-Si and Mg-Mg, how to explain this phenomenon?

Response 6: The reason why the average length of the Mg-Si bonds is shorter than that of the Mg-Mg and Si-Si is that the Si atoms were outwardly displaced. To clearly show the reason, we have added a sentence: "Therefore, the Si-Si bond is longer than the Mg-Si and the Mg-Mg bonds" In Lines: 140-141.

Point 7: In page 6, the authors performed the MC simulations, but not provide the details of the calculation settings, e.g. the time step ….

Response 7: We have performed not MD (Molecular Dynamics) but MC (Monte Carlo) calculations. Therefore, additional conditions such as the time step are not required.

Point 8: Some minor errors exist in some paragraphs/sentences and should be polished again carefully.

Response 8: We have checked and corrected minor errors.