We would like to thank the referees of Physical Review B for considering our paper for submission and giving us valuable suggestions. We have complied with the suggestions, and here is the summary of the improvements we have made to the paper and our response to the referees.

------------------------------------------------------------------------
Report of the First Referee -- BF12747/Talapatra
------------------------------------------------------------------------

The authors present an extensive ab-initio study of the transformations path in the martensitic Co2NiGa compound. They study all possible paths and show that the initial L21 structure may transform either to the L10 or the 0 structures. Although the O structure corresponds to lower total energy, several phenomena can lower the total energy of L10 and make it comparable to the one of the O structure. The latter has not been observed experimentally, and the authors suggest that there is very high energy barrier in the transformations path and, thus, Co2NiGa prefers the L10 structure.

The authors study is very broad covering an extended number of phenomena and paves the way for similar studies attacking the problem of martensitic phase transformations. Their study and results suggest that the investigation of such phenomena is very complex and a lot of possible alternatives should be taken into account. Experiments are useful and could be used as a guide for the theoretical studies trying to unveil the mechanisms between such phase transitions.

Moreover, the manuscript is well organized/written with adequate figures/tables/reference. I believe that it would be of extreme importance for scientists working on shape-memory-alloys and would serve as the prototype study for future research studies on these compounds.

We thank Referee # 1 for his appreciation of the work.

------------------------------------------------------------------------
Report of the Second Referee -- BF12747/Talapatra
------------------------------------------------------------------------

The authors present an excellent theoretical study of lower-symmetry allotropes of Co2NiGa. The topic is both very interesting and very important for possible future applications of this shape-memory material.
It is truly fascinating that the O phase is found energetically so much preferred over the L1_0 phase and the authors did an excellent job when trying to explain this issue. The paper should certainly be published but the authors should, in my opinion, introduce a series of changes as described below.

*First, the authors change local magnetic moments using a "MAGMOM" but  never really discuss the actual local magnetic moments in different phases. By the way, the term paramagnetic certainly does not mean zero local magnetic moments as in non-magnetic VASP calculations!*

We have used the fixed spin method in this work to approximately simulate magnetic disorder in the system. Specifically, we assign a value to the parameter 'NUPDOWN' in the INCAR file. Fixing the value of this parameter ensures that the difference of the number of electrons in the up and down spin component will be kept fixed to the specified value. We calculate the bain and burgers paths for the different values of NUPDOWN. For these calculations, VASP automatically sets MAGMOM = NUPDOWN/number of ions, hence we use the term 'MAGMOM' to denote the different cases. We have included an explanation in the revised manuscript. The authors did not detect any significant variation in the local magnetic moments and offer no insight and hence no discussion was included.

We agree, that we have used the term 'paramagnetic' inaccurately in the manuscript. The occurrences of 'paramagnetic' have been replaced with 'non-magnetic' or removed from the paper. In principle, we could use the disordered local moment method to simulate a somewhat paramagnetic state within VASP, but those calculations are outside the scope of this work.

*Second, when using the SQS, the symmetry is lowered and both studied paths (the Bain's and Burger's) are no longer identical when performed along different crystallographic directions. Are the changes significant? If yes, which results are depicted in Fig. 10?*

In the case of figure 10, i.e. the off-stoichiometric case, we used the SQS structure for the Bain path calculations only. This was not made evident in the paper. The Bain path (varying of c/a) was calculated for 2 cases: i) c || z and ii) c || y. We then selected the lower of the two bain paths.
For the Burgers path, we used a simple 16 atom supercell to simulate the $Co_{43.75}Ni_{25}Ga_{31.25}$ structure. Since Ga replaces Co, we considered all possible configurations and then selected the lowest energy configuration. The Burgers path was carried out on the lowest energy structure.
By this method, we used the lowest possible bain path and burgers paths, which encapsulate all possible energy ranges which may be observed and enable us to make a qualitative, if not quantitative observation.
An explanatory note has been included in the relevant section.

*Next, can the authors describe more in detail the way they computed the phonons? Which method was used? Now, having the phonon densities of states, would the authors consider computing a free energy of L21, L10 and O phases (by adding vibrational contribution to the free energy to the total energy differences that they present)? Would the energy order still be as in case of "bare" total energies presented in Table I?*

We include the following text in the manuscript:
'We use the fitfc module as implemented in the ATAT package to perform the vibrational calculations. This method consists of slightly perturbing the positions of the atoms away from their equilibrium position and calculating the reaction forces by fitting a spring model. Equating the calculated forces to the forces predicted from the harmonic model yields a set of linear constraints that allows the unknown force constants to be determined. The

force constant matrix is then used to extract the phonon density of states (pvdos) and the dispersion curves. Finally, we integrate the pvdos to calculate the vibrational contribution to the energy. '

The vibrational contribution to the free energy does not change the energy order as presented in Table I. The contribution is negligible (< 5 meV) and was hence not included in the work. A sentence has been added in Section V.B.1 to reflect this.

How do the authors define the volumetric strain energy?

We use a crude approximation to gain an insight into the energetics associated with volume change and use the following equation to calculate volumetric strain energy (Ev)

$$Ev = \frac{1}{2} * volumetric\ stress * volumetric\ strain$$

$$= \frac{1}{2} * (bulk\ modulus * volumetric\ strain) * \ volumetric\ strain$$

We have included the expression in the manuscript.

Lastly, would it be possible to consider all degrees of freedom in the
O phase and couple them all linearly so as to connect the O phase with
 (i) the L2_1 phase or
 (ii) L1_0 phase
in order to get at least a rough estimate of the energy barriers
schematically depicted in Fig. 5?

The authors use Fig.5 to drive the discussion and put forth the question of phase selection. Over the course of the analysis work carried out, it is seen that magnetic disorder/effect of temperature results in a lower energy for the L10 phase w.r.t the O phase, both being barrierless transformations. Hence, the L21-O path does not necessarily incur a higher barrier than that of L21-L10.
The authors did attempt to carry out a solid state nudged elastic band (NEB) calculation for the
i)  L21-O,
ii)  L21-L10 and
iii) L10-O paths.

While the NEB for the L21-L10 reproduced the bain path, the NEB paths for the other two transformations (L21-O and L10-O) did not converge. We suspect the vastly different unit cells in the transformation (the transformation being 2 dimensional) renders questionable the use of a linear interpolation technique to estimate intermediate states.

Finally, the authors thank Referee #2 for his valuable suggestions. We believe they have added necessary detail and clarity to this work.